Full wwPDB X-ray Structure Validation Report (i)

Dec 15, 2024 – 10:26 PM EST

PDB ID	:	4DL1
Title	:	Crystal Structure of human Myeloperoxidase with covalent thioxanthine analog
Authors	:	Vajdos, F.; Varghese, A.
Deposited on	:	2012-02-05
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

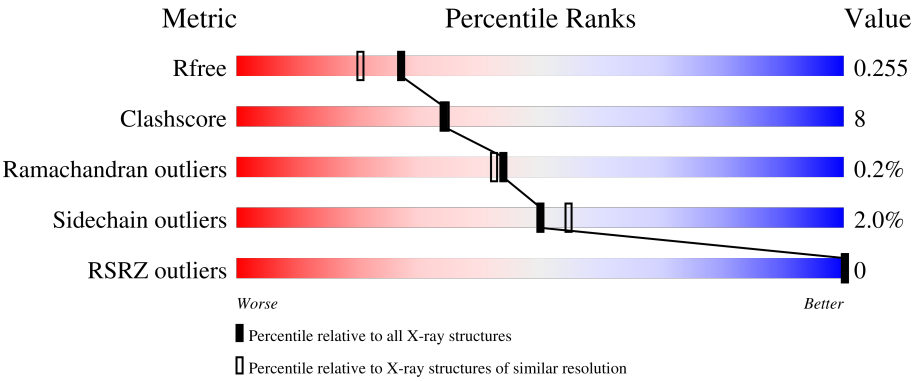
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	104	91% 9%
1	B	104	83% 17%
1	E	104	81% 19%
1	F	104	78% 21%
1	I	104	83% 15%

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Mol	Chain	Length	Quality of chain
1	J	104	93% 6%
1	M	104	85% 14%
1	N	104	85% 15%
2	C	466	86% 13%
2	D	466	86% 13%
2	G	466	80% 18%
2	H	466	85% 15%
2	K	466	84% 15%
2	L	466	86% 13%
2	O	466	82% 17%
2	P	466	85% 14%
3	Q	6	33% 50% 17%
3	R	6	33% 67%
3	S	6	33% 67%
3	T	6	33% 50% 17%
3	U	6	50% 50%
3	V	6	100%
3	W	6	17% 83%
3	X	6	83% 17%
4	Y	5	60% 40%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 40392 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Myeloperoxidase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	B	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	E	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	F	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	I	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	J	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	M	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	N	104	Total	C	N	O	S	0	1	0
			841	531	148	157	5			

- Molecule 2 is a protein called Myeloperoxidase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	465	Total	C	N	O	S	0	1	0
			3726	2348	686	665	27			
2	D	466	Total	C	N	O	S	0	0	0
			3729	2349	687	666	27			
2	G	465	Total	C	N	O	S	0	0	0
			3727	2348	686	666	27			
2	H	466	Total	C	N	O	S	0	0	0
			3729	2349	687	666	27			
2	K	465	Total	C	N	O	S	0	0	0
			3727	2348	686	666	27			
2	L	466	Total	C	N	O	S	0	0	0
			3730	2350	686	667	27			

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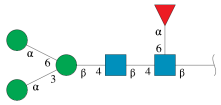
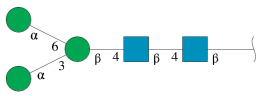
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	466	Total	C	N	O	S	0	0	0
			3729	2349	687	666	27			
2	P	466	Total	C	N	O	S	0	0	0
			3733	2351	687	668	27			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	R	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	S	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	T	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	U	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	V	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	W	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	X	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 4 is an oligosaccharide called 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.

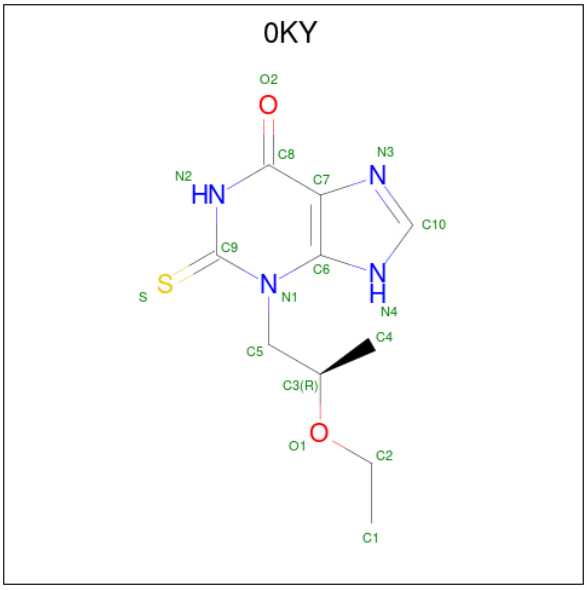


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Y	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0
5	I	1	Total Cl 1 1	0	0
5	J	1	Total Cl 1 1	0	0
5	M	1	Total Cl 1 1	0	0
5	N	1	Total Cl 1 1	0	0

- Molecule 6 is 3-[(2R)-2-ethoxypropyl]-2-thioxo-1,2,3,9-tetrahydro-6H-purin-6-one (three-letter code: 0KY) (formula: $C_{10}H_{14}N_4O_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O S 17 10 4 2 1	0	0
6	D	1	Total C N O S 17 10 4 2 1	0	0

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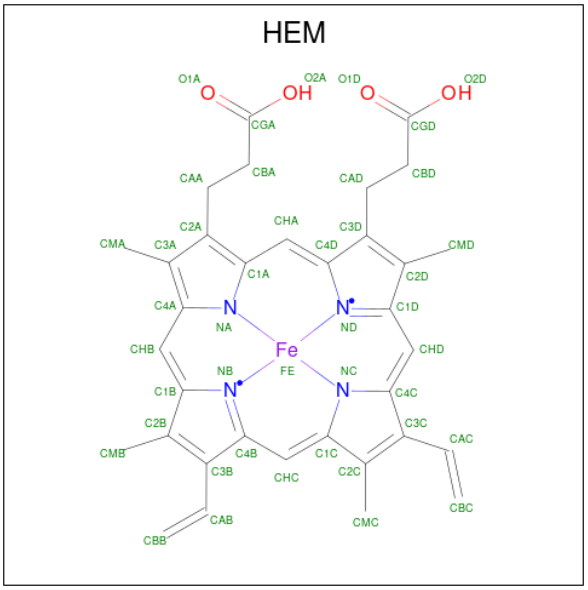
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	G	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
6	H	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
6	K	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
6	L	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
6	O	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
6	P	1	Total	C	N	O	S	0	0
			17	10	4	2	1		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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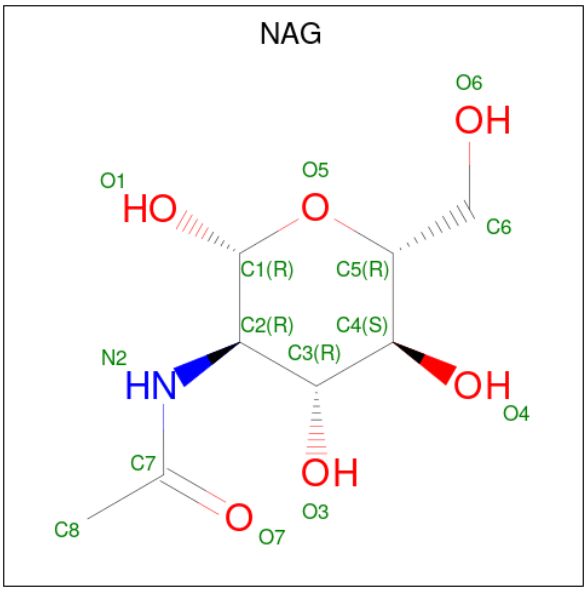
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O		0	0
			14	8	1	5			
8	C	1	Total	C	N	O		0	0
			14	8	1	5			
8	D	1	Total	C	N	O		0	0
			14	8	1	5			
8	D	1	Total	C	N	O		0	0
			14	8	1	5			
8	G	1	Total	C	N	O		0	0
			14	8	1	5			
8	G	1	Total	C	N	O		0	0
			14	8	1	5			
8	H	1	Total	C	N	O		0	0
			14	8	1	5			
8	H	1	Total	C	N	O		0	0
			14	8	1	5			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	K	1	Total C N O 14 8 1 5	0	0
8	K	1	Total C N O 14 8 1 5	0	0
8	L	1	Total C N O 14 8 1 5	0	0
8	L	1	Total C N O 14 8 1 5	0	0
8	O	1	Total C N O 14 8 1 5	0	0
8	O	1	Total C N O 14 8 1 5	0	0
8	P	1	Total C N O 14 8 1 5	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Ca 1 1	0	0
9	D	1	Total Ca 1 1	0	0
9	G	1	Total Ca 1 1	0	0
9	H	1	Total Ca 1 1	0	0
9	K	1	Total Ca 1 1	0	0
9	L	1	Total Ca 1 1	0	0
9	O	1	Total Ca 1 1	0	0
9	P	1	Total Ca 1 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	81	Total O 81 81	0	0
10	C	340	Total O 340 340	0	0

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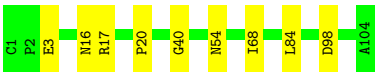
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	74	Total O 74 74	0	0
10	D	271	Total O 271 271	0	0
10	E	64	Total O 64 64	0	0
10	G	243	Total O 243 243	0	0
10	F	73	Total O 73 73	0	0
10	H	199	Total O 199 199	0	0
10	I	72	Total O 72 72	0	0
10	K	214	Total O 214 214	0	0
10	J	66	Total O 66 66	0	0
10	L	252	Total O 252 252	0	0
10	M	67	Total O 67 67	0	0
10	O	227	Total O 227 227	0	0
10	N	62	Total O 62 62	0	0
10	P	215	Total O 215 215	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Myeloperoxidase light chain

Chain A:

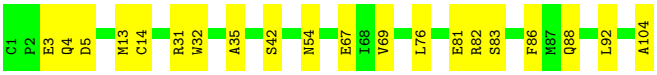


• Molecule 1: Myeloperoxidase light chain

Chain B:

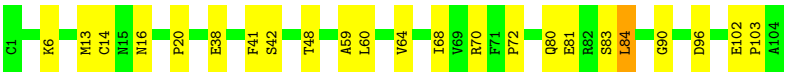
• Molecule 1: Myeloperoxidase light chain

Chain E:



• Molecule 1: Myeloperoxidase light chain

Chain F:



• Molecule 1: Myeloperoxidase light chain

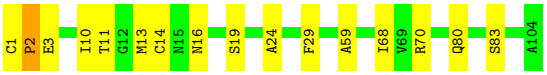
Chain I:

• Molecule 1: Myeloperoxidase light chain

Chain J:

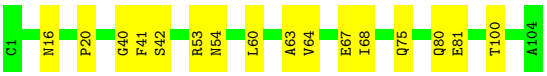
• Molecule 1: Myeloperoxidase light chain

Chain M:



• Molecule 1: Myeloperoxidase light chain

Chain N:

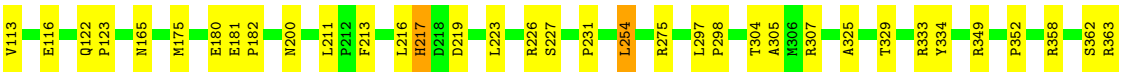


• Molecule 2: Myeloperoxidase heavy chain

Chain C:

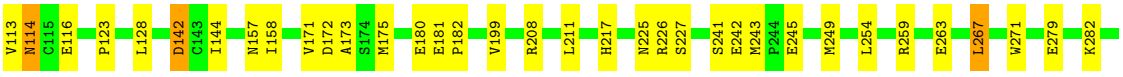
• Molecule 2: Myeloperoxidase heavy chain

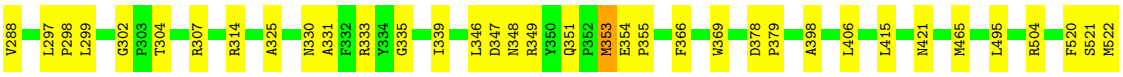
Chain D:

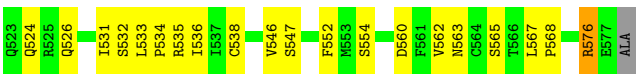


• Molecule 2: Myeloperoxidase heavy chain

Chain G:

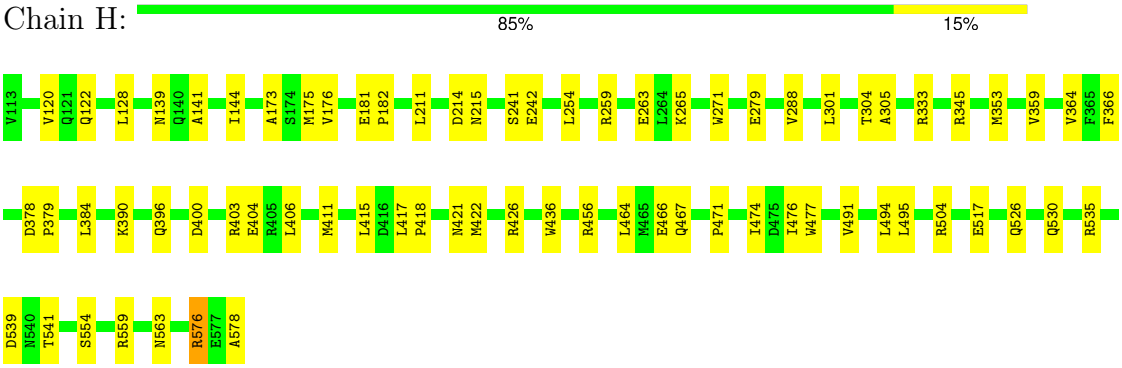






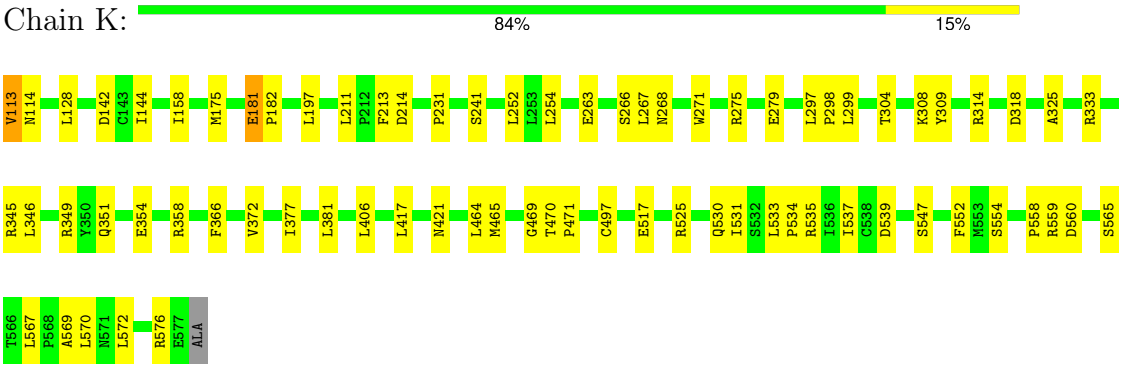
• Molecule 2: Myeloperoxidase heavy chain

Chain H:



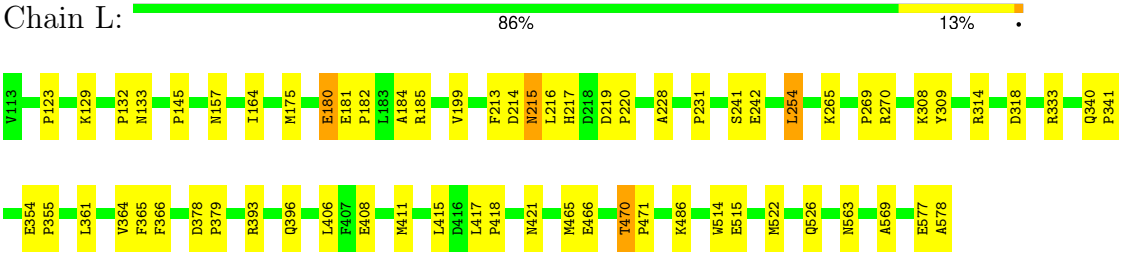
• Molecule 2: Myeloperoxidase heavy chain

Chain K:



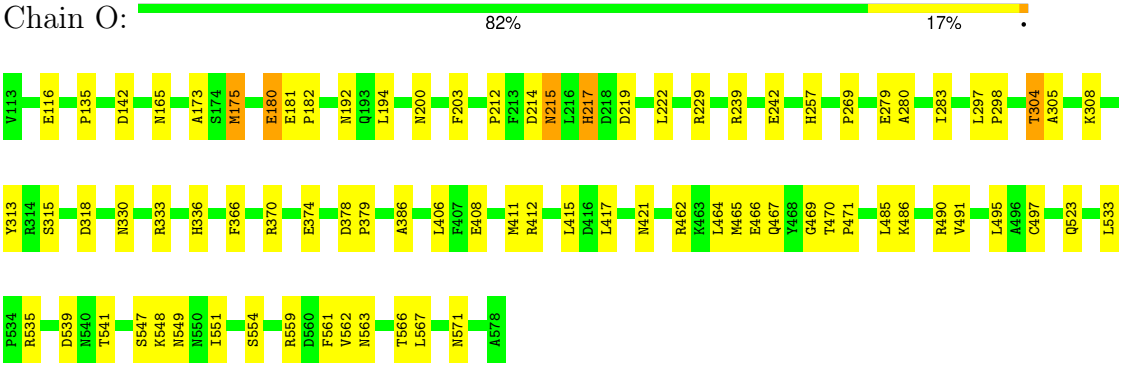
• Molecule 2: Myeloperoxidase heavy chain

Chain L:



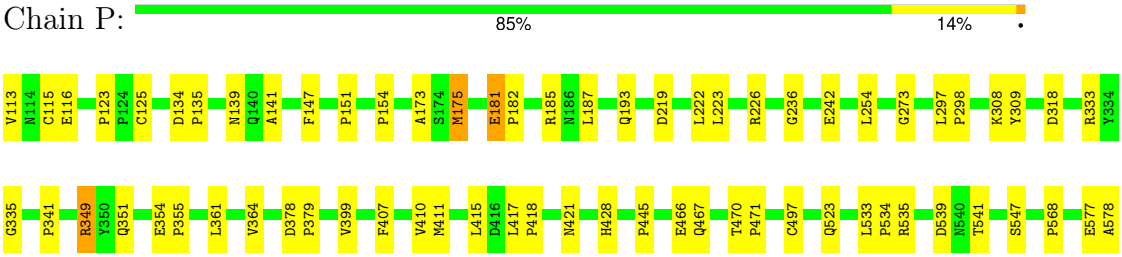
• Molecule 2: Myeloperoxidase heavy chain

Chain O:



• Molecule 2: Myeloperoxidase heavy chain

Chain P:



• Molecule 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

• Molecule 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

• Molecule 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

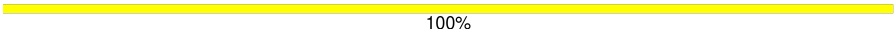
Chain T:

• Molecule 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

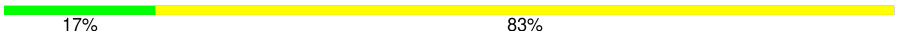
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



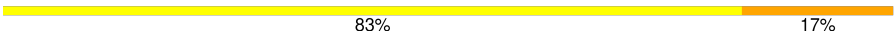
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



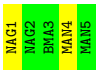
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



• Molecule 4: 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

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.83Å 242.64Å 151.50Å 90.00° 91.19° 90.00°	Depositor
Resolution (Å)	128.49 – 2.00 128.49 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (128.49-2.00) 97.6 (128.49-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.246 0.204 , 0.255	Depositor DCC
R_{free} test set	15173 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 28.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	40392	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5328e-03.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, NAG, CSO, MAN, BMA, 0KY, CL, FUC, HEM

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	0.58	0/863	0.69	0/1174
1	B	0.53	0/863	0.61	0/1174
1	E	0.58	0/863	0.63	0/1174
1	F	0.47	0/863	0.59	0/1174
1	I	0.52	0/863	0.61	0/1174
1	J	0.49	0/863	0.59	0/1174
1	M	0.47	0/863	0.58	0/1174
1	N	0.47	0/869	0.57	0/1183
2	C	0.58	0/3807	0.61	0/5164
2	D	0.51	0/3807	0.57	0/5163
2	G	0.51	0/3805	0.58	0/5161
2	H	0.44	0/3807	0.53	0/5163
2	K	0.48	0/3805	0.55	0/5161
2	L	0.48	0/3808	0.56	1/5164 (0.0%)
2	O	0.45	0/3807	0.54	0/5163
2	P	0.45	0/3811	0.52	0/5168
All	All	0.50	0/37367	0.57	1/50708 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
2	D	0	1
2	G	0	2
2	K	0	1
2	L	0	1
2	O	0	3
All	All	0	9

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	318	ASP	CB-CG-OD1	5.26	123.03	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	180	GLU	Peptide
2	G	180	GLU	Peptide
2	G	302	GLY	Peptide
1	I	2	PRO	Peptide
2	K	547	SER	Peptide
2	L	180	GLU	Peptide
2	O	180	GLU	Peptide
2	O	214	ASP	Peptide
2	O	215	ASN	Peptide

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	838	0	798	9	0
1	B	838	0	798	18	0
1	E	838	0	798	16	0
1	F	838	0	798	27	0
1	I	838	0	798	18	0
1	J	838	0	798	5	0
1	M	838	0	798	11	0
1	N	841	0	803	11	0
2	C	3726	0	3721	63	0
2	D	3729	0	3721	45	0
2	G	3727	0	3720	69	1
2	H	3729	0	3721	70	0
2	K	3727	0	3720	48	0
2	L	3730	0	3721	47	0
2	O	3729	0	3721	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	3733	0	3725	56	0
3	Q	71	0	61	1	0
3	R	71	0	61	0	0
3	S	71	0	61	0	0
3	T	71	0	61	1	0
3	U	71	0	61	0	0
3	V	71	0	61	0	0
3	W	71	0	61	1	0
3	X	71	0	61	2	0
4	Y	61	0	52	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
6	C	17	0	14	3	0
6	D	17	0	14	4	0
6	G	17	0	14	1	0
6	H	17	0	14	5	0
6	K	17	0	14	2	0
6	L	17	0	14	1	0
6	O	17	0	14	5	0
6	P	17	0	14	4	0
7	C	43	0	30	6	0
7	D	43	0	30	5	0
7	G	43	0	30	6	0
7	H	43	0	30	5	0
7	K	43	0	30	1	0
7	L	43	0	30	5	0
7	O	43	0	30	5	0
7	P	43	0	30	7	0
8	C	28	0	26	0	0
8	D	28	0	26	1	0
8	G	28	0	26	2	0
8	H	28	0	26	0	0
8	K	28	0	26	0	0
8	L	28	0	26	0	0
8	O	28	0	26	0	0
8	P	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0
9	O	1	0	0	0	0
9	P	1	0	0	0	0
10	A	81	0	0	1	0
10	B	74	0	0	0	0
10	C	340	0	0	16	0
10	D	271	0	0	10	0
10	E	64	0	0	4	0
10	F	73	0	0	1	0
10	G	243	0	0	16	0
10	H	199	0	0	11	0
10	I	72	0	0	1	0
10	J	66	0	0	1	0
10	K	214	0	0	9	0
10	L	252	0	0	11	1
10	M	67	0	0	2	0
10	N	62	0	0	1	0
10	O	227	0	0	18	0
10	P	215	0	0	12	0
All	All	40392	0	37246	566	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 8.

All (566) 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)
2:C:465:MET:CE	2:C:471:PRO:HG3	1.79	1.12
1:N:63:ALA:O	1:N:67:GLU:HG2	1.50	1.09
1:F:84:LEU:HD22	2:H:384:LEU:HD23	1.35	1.09
2:C:465:MET:HE3	2:C:471:PRO:HD3	1.34	1.05
2:P:116:GLU:OE2	2:P:411:MET:HE3	1.57	1.05
2:C:465:MET:HE1	2:C:471:PRO:CG	1.87	1.04
2:C:465:MET:HE1	2:C:471:PRO:HG3	1.04	1.04
1:F:84:LEU:CD2	2:H:384:LEU:HD23	1.94	0.96
2:H:214:ASP:HB3	10:H:712:HOH:O	1.66	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:173:ALA:HA	2:H:175:MET:HE3	1.49	0.92
2:O:465:MET:HE1	2:O:470:THR:HA	1.54	0.89
2:G:211:LEU:HD23	2:G:254:LEU:HD13	1.55	0.88
2:C:347:ASP:HB2	1:I:80:GLN:OE1	1.72	0.88
2:C:465:MET:HE3	2:C:471:PRO:CD	2.05	0.87
7:H:601:HEM:HMC2	7:H:601:HEM:HBC2	1.57	0.86
2:C:465:MET:CE	2:C:471:PRO:CG	2.48	0.86
2:P:411:MET:HE1	2:P:415:LEU:HD21	1.59	0.83
2:C:531:ILE:C	2:C:531:ILE:HD12	1.98	0.82
2:G:113:VAL:HG12	2:G:113:VAL:O	1.80	0.81
2:O:200:ASN:HD22	2:O:203:PHE:H	1.27	0.81
2:D:577:GLU:O	2:D:578:ALA:HB3	1.81	0.81
2:C:465:MET:CE	2:C:471:PRO:HD3	2.12	0.80
1:I:16:ASN:HD22	1:I:19:SER:H	1.29	0.80
1:F:84:LEU:CD2	2:H:384:LEU:CD2	2.60	0.79
2:L:181:GLU:OE2	2:L:181:GLU:O	2.01	0.79
1:N:64:VAL:HG13	1:N:68:ILE:HD12	1.63	0.79
2:H:175:MET:CE	2:H:288:VAL:HG11	2.13	0.78
2:O:411:MET:HE2	2:O:415:LEU:HD21	1.64	0.78
1:B:6:LYS:NZ	2:D:275:ARG:NH2	2.31	0.78
6:O:605:0KY:H8	10:O:912:HOH:O	1.84	0.78
2:P:116:GLU:OE2	2:P:411:MET:CE	2.31	0.78
2:C:465:MET:CE	2:C:471:PRO:CD	2.61	0.78
2:D:577:GLU:O	2:D:578:ALA:CB	2.32	0.78
2:G:181:GLU:N	2:G:182:PRO:HD2	1.99	0.77
2:C:348:ASN:ND2	1:I:77:THR:CG2	2.48	0.77
2:K:535:ARG:NH1	2:K:567:LEU:O	2.19	0.76
1:F:64:VAL:CG1	1:F:68:ILE:HD12	2.15	0.76
1:M:83:SER:HB3	2:O:554:SER:O	1.85	0.76
2:H:504:ARG:HB3	10:H:868:HOH:O	1.84	0.76
1:F:38:GLU:OE1	1:F:48:THR:OG1	2.04	0.75
2:H:181:GLU:N	2:H:182:PRO:HD2	2.02	0.75
2:C:486:LYS:HE3	10:C:730:HOH:O	1.86	0.75
2:H:120:VAL:HG12	2:H:122:GLN:HG3	1.68	0.75
2:H:175:MET:HE2	2:H:288:VAL:HG11	1.67	0.75
1:F:84:LEU:HD23	2:H:384:LEU:CD2	2.17	0.74
10:J:315:HOH:O	2:L:129:LYS:HE3	1.87	0.73
2:C:304:THR:HG22	10:C:991:HOH:O	1.87	0.73
2:P:113:VAL:HG13	2:P:113:VAL:O	1.86	0.73
2:O:304:THR:HG22	10:O:861:HOH:O	1.87	0.73
2:P:577:GLU:O	2:P:578:ALA:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:466:GLU:OE1	10:P:701:HOH:O	2.05	0.73
2:C:488:LYS:HD2	10:C:743:HOH:O	1.90	0.72
7:C:602:HEM:HMC2	7:C:602:HEM:HBC2	1.72	0.72
2:O:333:ARG:HH11	2:O:421:ASN:HD22	1.37	0.72
7:P:601:HEM:HAA2	6:P:604:0KY:S	2.29	0.72
7:D:601:HEM:HBA1	6:D:602:0KY:S	2.30	0.71
2:K:465:MET:HE1	2:K:471:PRO:HD3	1.72	0.71
1:B:6:LYS:NZ	2:D:275:ARG:HH21	1.88	0.71
2:G:349:ARG:HG3	2:G:351:GLN:HG2	1.72	0.70
1:M:16:ASN:HD22	1:M:19:SER:H	1.37	0.70
2:G:333:ARG:HH11	2:G:421:ASN:HD22	1.39	0.70
7:L:601:HEM:HBC2	7:L:601:HEM:HMC2	1.72	0.69
2:C:348:ASN:ND2	1:I:77:THR:HG23	2.08	0.69
2:L:242:GLU:OE1	7:L:601:HEM:HBB2	1.91	0.69
1:M:68:ILE:HD13	2:O:464:LEU:HD23	1.74	0.68
2:D:352:PRO:HD2	10:D:893:HOH:O	1.93	0.68
2:P:182:PRO:HG2	10:P:878:HOH:O	1.94	0.68
2:O:217:HIS:HE1	10:O:909:HOH:O	1.77	0.68
7:G:601:HEM:HBC2	7:G:601:HEM:HMC2	1.75	0.68
2:K:465:MET:HE1	2:K:470:THR:HA	1.75	0.68
2:L:411:MET:CE	2:L:415:LEU:HD21	2.23	0.68
1:E:67:GLU:OE1	1:E:67:GLU:HA	1.95	0.67
7:H:601:HEM:HBC2	7:H:601:HEM:CMC	2.23	0.67
2:D:181:GLU:N	2:D:182:PRO:HD2	2.10	0.67
2:O:559:ARG:HD3	10:O:862:HOH:O	1.95	0.67
6:H:605:0KY:H11	6:H:605:0KY:C6	2.24	0.66
1:F:64:VAL:HG13	1:F:68:ILE:HD12	1.76	0.66
2:G:531:ILE:C	2:G:531:ILE:HD12	2.15	0.66
2:L:157:ASN:HB2	10:L:913:HOH:O	1.94	0.66
2:H:406:LEU:HD22	2:H:417:LEU:HB2	1.77	0.66
2:K:465:MET:HE3	10:K:752:HOH:O	1.94	0.66
2:C:270:ARG:HG3	10:C:1008:HOH:O	1.95	0.66
2:H:436:TRP:CD1	2:H:476:ILE:HD13	2.30	0.66
2:L:123:PRO:HA	10:L:934:HOH:O	1.95	0.65
2:P:378:ASP:HB2	2:P:379:PRO:HD3	1.77	0.65
1:I:68:ILE:HD13	2:K:464:LEU:HD23	1.78	0.65
2:K:113:VAL:HA	10:K:826:HOH:O	1.95	0.65
2:O:333:ARG:HH11	2:O:421:ASN:ND2	1.94	0.65
2:G:333:ARG:HH11	2:G:421:ASN:ND2	1.93	0.65
2:P:113:VAL:HG13	2:P:125:CYS:SG	2.36	0.64
2:C:116:GLU:OE1	2:C:411:MET:CE	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HD13	2:D:389:ALA:HA	1.80	0.64
7:P:601:HEM:HMC2	7:P:601:HEM:HBC2	1.78	0.64
2:P:181:GLU:HG2	10:P:726:HOH:O	1.97	0.64
2:C:486:LYS:CE	10:C:730:HOH:O	2.45	0.64
2:G:331:ALA:HB1	2:G:495:LEU:HD23	1.80	0.64
2:O:563:ASN:HB3	10:O:866:HOH:O	1.98	0.64
2:O:567:LEU:N	2:O:567:LEU:HD23	2.13	0.64
2:P:123:PRO:HA	10:P:875:HOH:O	1.98	0.63
2:G:353:MET:HG2	10:G:883:HOH:O	1.98	0.63
1:N:16:ASN:O	1:N:20:PRO:HA	1.97	0.63
2:H:301:LEU:HB3	2:H:305:ALA:HB3	1.81	0.63
6:C:601:0KY:H11	6:C:601:0KY:C6	2.29	0.63
2:P:242:GLU:HG3	6:P:604:0KY:O2	1.98	0.63
10:G:943:HOH:O	3:T:4:MAN:H61	1.98	0.63
7:P:601:HEM:HBB2	7:P:601:HEM:HMB1	1.80	0.62
2:P:113:VAL:O	2:P:113:VAL:CG1	2.47	0.62
2:O:523:GLN:HG2	10:O:922:HOH:O	1.99	0.62
6:H:605:0KY:H11	6:H:605:0KY:N4	2.15	0.62
2:C:531:ILE:HD12	2:C:531:ILE:O	1.98	0.62
7:D:601:HEM:HBC2	7:D:601:HEM:HMC2	1.80	0.62
1:F:64:VAL:HG12	1:F:68:ILE:HD12	1.82	0.62
1:M:70:ARG:CZ	10:M:1707:HOH:O	2.48	0.62
2:H:211:LEU:HD23	2:H:254:LEU:HD22	1.82	0.61
2:O:559:ARG:CD	10:O:862:HOH:O	2.49	0.61
2:H:411:MET:HE2	2:H:415:LEU:HD21	1.82	0.61
2:C:181:GLU:N	2:C:182:PRO:CD	2.63	0.61
2:P:535:ARG:NH2	2:P:539:ASP:OD2	2.32	0.61
2:K:211:LEU:HD23	2:K:254:LEU:HD22	1.82	0.61
8:G:603:NAG:O7	8:G:603:NAG:O3	2.15	0.60
2:P:354:GLU:OE1	2:P:355:PRO:O	2.18	0.60
2:G:123:PRO:HA	10:G:931:HOH:O	2.02	0.60
2:O:239:ARG:HG2	6:O:605:0KY:N3	2.17	0.60
2:P:151:PRO:HG2	2:P:154:PRO:HG3	1.84	0.60
1:I:16:ASN:ND2	1:I:19:SER:H	1.99	0.59
2:K:181:GLU:N	2:K:182:PRO:CD	2.66	0.59
2:H:411:MET:CE	2:H:415:LEU:HD21	2.32	0.59
2:D:200:ASN:HB2	2:D:211:LEU:O	2.02	0.59
2:H:259:ARG:O	2:H:263:GLU:HG3	2.03	0.59
2:O:181:GLU:N	2:O:182:PRO:CD	2.66	0.59
2:O:548:LYS:HZ3	2:O:562:VAL:CG1	2.15	0.59
2:K:263:GLU:O	2:K:266:SER:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:411:MET:CE	2:P:415:LEU:HD21	2.30	0.59
2:G:181:GLU:H	2:G:182:PRO:HD2	1.66	0.58
2:L:569:ALA:HB3	10:L:743:HOH:O	2.03	0.58
7:O:601:HEM:HBC2	7:O:601:HEM:HMC2	1.84	0.58
2:P:193:GLN:NE2	2:P:273:GLY:H	2.01	0.58
1:E:104:ALA:HA	10:E:1715:HOH:O	2.01	0.58
1:B:6:LYS:HZ3	2:D:275:ARG:HH21	1.50	0.58
1:F:96:ASP:OD2	2:H:175:MET:HE2	2.03	0.58
2:G:113:VAL:O	2:G:113:VAL:CG1	2.50	0.58
1:F:70:ARG:HH11	2:H:403:ARG:NH2	2.02	0.58
2:H:422:MET:O	2:H:426:ARG:HG3	2.04	0.58
7:G:601:HEM:HBC2	7:G:601:HEM:CMC	2.34	0.58
2:P:308:LYS:HE3	3:W:4:MAN:O2	2.03	0.58
2:C:211:LEU:HD23	2:C:254:LEU:HD13	1.85	0.58
2:C:377:ILE:HD12	2:C:381:LEU:HD11	1.86	0.57
2:D:116:GLU:OE2	2:D:411:MET:HE3	2.04	0.57
2:H:175:MET:HE1	2:H:288:VAL:HG21	1.85	0.57
2:P:115:CYS:HB2	2:P:147:PHE:CE1	2.39	0.57
2:O:366:PHE:CZ	6:O:605:0KY:H9	2.40	0.57
2:D:333:ARG:HH11	2:D:421:ASN:HD22	1.53	0.57
2:L:157:ASN:CB	10:L:913:HOH:O	2.50	0.57
2:C:522:MET:HE2	10:P:910:HOH:O	2.04	0.57
2:O:465:MET:CE	2:O:469:GLY:O	2.53	0.57
2:K:531:ILE:HD12	2:K:531:ILE:C	2.25	0.57
2:C:116:GLU:OE1	2:C:411:MET:HE3	2.05	0.57
2:C:576:ARG:HD2	10:C:941:HOH:O	2.04	0.57
2:H:576:ARG:CG	2:H:578:ALA:HB2	2.35	0.57
1:A:68:ILE:HD13	2:C:464:LEU:HD23	1.86	0.57
2:G:211:LEU:CD2	2:G:254:LEU:HD13	2.30	0.57
2:L:411:MET:HE2	2:L:415:LEU:HD21	1.86	0.56
2:C:219:ASP:HB3	2:C:222:LEU:HD12	1.87	0.56
2:G:171:VAL:CG1	2:G:288:VAL:HG12	2.35	0.56
1:M:16:ASN:ND2	1:M:19:SER:H	2.03	0.56
2:D:488:LYS:HD2	10:D:937:HOH:O	2.06	0.56
2:H:120:VAL:CG1	2:H:122:GLN:HG3	2.34	0.56
2:G:335:GLY:HA3	7:G:601:HEM:CBC	2.35	0.56
1:F:68:ILE:HD13	2:H:464:LEU:HD23	1.86	0.56
2:K:271:TRP:CZ3	2:K:279:GLU:HG3	2.39	0.56
1:I:13:MET:O	1:I:14:CYS:HB2	2.05	0.56
10:M:1707:HOH:O	2:O:135:PRO:HG3	2.04	0.56
2:O:200:ASN:ND2	2:O:203:PHE:H	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:465:MET:HE3	10:O:814:HOH:O	2.05	0.56
2:L:314:ARG:HG2	10:L:800:HOH:O	2.06	0.55
2:P:182:PRO:CG	10:P:890:HOH:O	2.54	0.55
2:L:216:LEU:HD13	2:L:219:ASP:OD1	2.06	0.55
2:D:181:GLU:N	2:D:182:PRO:CD	2.68	0.55
2:O:386:ALA:HB2	2:O:561:PHE:CZ	2.40	0.55
2:D:333:ARG:HH11	2:D:421:ASN:ND2	2.04	0.55
2:G:226:ARG:HD3	10:G:937:HOH:O	2.06	0.55
2:G:378:ASP:HB2	2:G:379:PRO:HD3	1.89	0.55
1:A:54:ASN:HB2	10:A:1757:HOH:O	2.06	0.55
1:I:5:ASP:OD1	1:I:5:ASP:N	2.40	0.55
7:P:601:HEM:CAA	6:P:604:0KY:S	2.95	0.55
2:D:382:ARG:NH2	10:D:701:HOH:O	2.25	0.55
2:G:181:GLU:N	2:G:182:PRO:CD	2.68	0.55
2:K:268:ASN:OD1	2:K:576:ARG:HA	2.07	0.54
1:E:54:ASN:CB	10:E:1749:HOH:O	2.54	0.54
2:C:531:ILE:C	2:C:531:ILE:CD1	2.70	0.54
2:G:331:ALA:HB1	2:G:495:LEU:CD2	2.37	0.54
2:C:121:GLN:NE2	10:C:705:HOH:O	2.40	0.54
2:K:142:ASP:HB3	10:K:858:HOH:O	2.07	0.54
2:O:465:MET:HE3	2:O:469:GLY:O	2.07	0.54
2:C:120:VAL:HG12	2:C:122:GLN:HG2	1.90	0.54
1:J:56:PHE:CD2	2:L:470:THR:HG22	2.43	0.54
2:P:407:PHE:O	2:P:410:VAL:HG22	2.08	0.54
2:G:533:LEU:HB3	2:G:534:PRO:HD3	1.90	0.54
2:L:361:LEU:HA	2:L:364:VAL:HG22	1.89	0.54
2:C:133:ASN:HB3	2:H:517:GLU:OE2	2.08	0.54
2:G:521:SER:OG	2:G:524:GLN:HG3	2.08	0.53
1:F:102:GLU:HB3	1:F:103:PRO:HD2	1.89	0.53
2:C:333:ARG:HH11	2:C:421:ASN:HD22	1.56	0.53
10:O:913:HOH:O	3:X:4:MAN:H62	2.08	0.53
1:A:68:ILE:CD1	2:C:464:LEU:HD23	2.38	0.53
1:N:63:ALA:O	1:N:67:GLU:CG	2.41	0.53
1:A:3:GLU:O	1:A:17:ARG:NH1	2.31	0.53
2:D:182:PRO:HG2	10:D:922:HOH:O	2.07	0.53
1:E:54:ASN:CG	10:E:1749:HOH:O	2.47	0.53
2:L:217:HIS:CE1	10:L:870:HOH:O	2.61	0.53
2:L:577:GLU:O	2:L:578:ALA:OXT	2.26	0.53
2:D:535:ARG:NH1	2:D:567:LEU:O	2.42	0.53
2:L:214:ASP:OD1	2:L:215:ASN:N	2.35	0.53
2:G:208:ARG:NH2	10:G:701:HOH:O	2.13	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:VAL:CG1	2:G:398:ALA:HB3	2.39	0.53
2:G:307:ARG:HD3	10:G:927:HOH:O	2.08	0.53
2:L:465:MET:SD	2:L:471:PRO:HD3	2.49	0.53
2:H:175:MET:HE1	2:H:288:VAL:HG11	1.88	0.52
1:I:54:ASN:HA	10:I:1712:HOH:O	2.10	0.52
2:L:214:ASP:HB3	2:L:216:LEU:CD1	2.40	0.52
2:O:485:LEU:HD13	2:O:490:ARG:HA	1.92	0.52
1:N:80:GLN:O	1:N:80:GLN:HG3	2.08	0.52
1:F:90:GLY:HA3	7:H:601:HEM:CBC	2.40	0.52
2:C:348:ASN:HD21	1:I:77:THR:HG22	1.74	0.52
2:G:406:LEU:HB3	2:G:415:LEU:HB2	1.92	0.52
2:H:181:GLU:H	2:H:182:PRO:HD2	1.72	0.52
2:C:348:ASN:HD21	1:I:77:THR:CG2	2.21	0.52
7:P:601:HEM:HBB2	7:P:601:HEM:CMB	2.40	0.52
2:H:333:ARG:HH11	2:H:421:ASN:HD22	1.57	0.52
2:P:568:PRO:HA	10:P:900:HOH:O	2.09	0.52
1:A:16:ASN:O	1:A:20:PRO:HA	2.10	0.51
2:C:114:ASN:HA	10:C:959:HOH:O	2.10	0.51
2:O:566:THR:C	2:O:567:LEU:HD23	2.30	0.51
2:P:417:LEU:HB3	2:P:418:PRO:HD3	1.92	0.51
2:G:267:LEU:HD13	2:G:576:ARG:HB2	1.93	0.51
2:C:244:PRO:HD3	2:C:364:VAL:O	2.10	0.51
2:G:354:GLU:OE1	2:G:354:GLU:HA	2.10	0.51
2:H:535:ARG:NH2	2:H:539:ASP:OD2	2.42	0.51
1:J:76:LEU:HD23	1:J:76:LEU:C	2.31	0.51
1:I:52:LYS:HD3	2:O:412:ARG:O	2.11	0.51
2:K:213:PHE:CD1	2:K:231:PRO:HG2	2.45	0.51
2:L:214:ASP:HB3	2:L:216:LEU:HD12	1.91	0.51
1:E:3:GLU:O	1:E:4:GLN:HB2	2.10	0.51
2:K:535:ARG:NH2	2:K:539:ASP:OD2	2.40	0.51
2:L:406:LEU:HD23	2:L:415:LEU:HB2	1.91	0.51
7:O:601:HEM:HBA1	6:O:605:0KY:S	2.51	0.51
1:F:70:ARG:HH11	2:H:403:ARG:HH21	1.57	0.51
2:O:378:ASP:HB2	2:O:379:PRO:HD3	1.92	0.51
1:F:16:ASN:O	1:F:20:PRO:HA	2.11	0.50
2:H:181:GLU:N	2:H:182:PRO:CD	2.71	0.50
2:G:113:VAL:O	2:G:114:ASN:C	2.50	0.50
2:H:333:ARG:HH11	2:H:421:ASN:ND2	2.08	0.50
2:L:340:GLN:OE1	2:L:341:PRO:HD2	2.12	0.50
2:D:307:ARG:NH1	10:D:704:HOH:O	2.44	0.50
2:G:128:LEU:HB2	2:G:144:ILE:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:267:LEU:CD2	10:G:914:HOH:O	2.59	0.50
1:F:72:PRO:HA	10:F:334:HOH:O	2.11	0.50
2:O:336:HIS:CE1	2:O:417:LEU:HD21	2.47	0.50
1:B:83:SER:HB3	2:D:554:SER:O	2.11	0.50
2:H:378:ASP:OD1	2:H:541:THR:HB	2.12	0.50
2:H:378:ASP:HB2	2:H:379:PRO:HD3	1.93	0.50
2:P:181:GLU:N	2:P:182:PRO:HD2	2.26	0.50
1:A:84:LEU:HD13	2:C:389:ALA:HA	1.94	0.50
2:C:488:LYS:CE	10:C:743:HOH:O	2.60	0.50
2:H:242:GLU:HG3	6:H:605:0KY:O2	2.12	0.50
1:A:98:ASP:OD2	7:C:602:HEM:O1D	2.30	0.50
7:C:602:HEM:CMB	7:C:602:HEM:HBB2	2.41	0.50
2:G:355:PRO:HD2	10:G:766:HOH:O	2.12	0.50
2:K:267:LEU:O	2:K:576:ARG:NH1	2.44	0.50
2:K:308:LYS:NZ	10:K:704:HOH:O	2.40	0.50
1:E:76:LEU:HD23	1:E:76:LEU:C	2.33	0.49
1:F:59:ALA:HB2	2:H:467:GLN:O	2.12	0.49
7:C:602:HEM:HBC2	7:C:602:HEM:CMC	2.40	0.49
2:H:563:ASN:ND2	10:H:707:HOH:O	2.45	0.49
2:O:192:ASN:CG	2:O:194:LEU:HD12	2.32	0.49
2:O:486:LYS:CE	10:O:884:HOH:O	2.59	0.49
1:N:67:GLU:HG3	2:P:467:GLN:NE2	2.27	0.49
7:P:601:HEM:HBC2	7:P:601:HEM:CMC	2.42	0.49
2:L:181:GLU:N	2:L:182:PRO:CD	2.75	0.49
1:B:16:ASN:O	1:B:20:PRO:HA	2.12	0.49
2:H:576:ARG:HG3	2:H:578:ALA:HB2	1.94	0.49
1:N:40:GLY:HA2	10:N:334:HOH:O	2.11	0.49
6:C:601:0KY:H2	10:C:782:HOH:O	2.11	0.49
2:K:372:VAL:O	10:K:701:HOH:O	2.20	0.49
2:K:525:ARG:HD3	10:K:754:HOH:O	2.12	0.49
2:P:577:GLU:O	2:P:578:ALA:C	2.50	0.49
2:C:559:ARG:HD2	10:C:1000:HOH:O	2.13	0.49
2:K:530:GLN:NE2	10:K:708:HOH:O	2.46	0.49
1:E:81:GLU:HG2	10:E:1758:HOH:O	2.12	0.49
2:H:417:LEU:HB3	2:H:418:PRO:HD3	1.95	0.49
1:M:1:CYS:O	1:M:2:PRO:C	2.51	0.49
2:P:219:ASP:HB3	2:P:222:LEU:HD12	1.95	0.49
6:P:604:0KY:H14	10:P:702:HOH:O	2.13	0.49
2:G:554:SER:HB3	2:G:560:ASP:HB3	1.94	0.49
1:J:16:ASN:O	1:J:20:PRO:HA	2.12	0.49
7:O:601:HEM:HMB1	7:O:601:HEM:HBB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:LEU:HB2	2:H:144:ILE:HB	1.94	0.48
2:H:353:MET:CE	10:H:711:HOH:O	2.60	0.48
2:O:269:PRO:HD2	10:O:855:HOH:O	2.12	0.48
2:C:116:GLU:OE1	2:C:411:MET:HE1	2.13	0.48
1:E:92:LEU:HD22	2:G:249:MET:HB3	1.94	0.48
1:N:41:PHE:CD1	1:N:42:SER:HB2	2.48	0.48
2:P:115:CYS:HB2	2:P:147:PHE:CZ	2.48	0.48
2:P:333:ARG:HH11	2:P:421:ASN:ND2	2.11	0.48
6:H:605:0KY:C6	6:H:605:0KY:C4	2.90	0.48
2:K:128:LEU:HB2	2:K:144:ILE:HB	1.94	0.48
2:L:216:LEU:HD22	2:L:220:PRO:HD2	1.95	0.48
2:L:569:ALA:CB	10:L:743:HOH:O	2.59	0.48
2:C:488:LYS:CD	10:C:743:HOH:O	2.57	0.48
7:C:602:HEM:HBB2	7:C:602:HEM:HMB1	1.95	0.48
2:O:465:MET:HE1	2:O:471:PRO:HD3	1.96	0.48
6:K:602:0KY:C6	6:K:602:0KY:H11	2.43	0.48
2:L:563:ASN:HB3	10:L:881:HOH:O	2.14	0.48
7:O:601:HEM:HBC2	7:O:601:HEM:CMC	2.43	0.48
2:C:333:ARG:HH11	2:C:421:ASN:ND2	2.11	0.48
2:G:348:ASN:OD1	2:G:349:ARG:N	2.46	0.48
2:H:182:PRO:HG2	10:H:857:HOH:O	2.14	0.48
7:O:601:HEM:HBB2	7:O:601:HEM:CMB	2.43	0.48
2:D:116:GLU:OE2	2:D:411:MET:CE	2.61	0.48
7:D:601:HEM:HBC2	7:D:601:HEM:CMC	2.43	0.48
2:H:345:ARG:NE	10:H:711:HOH:O	2.47	0.47
2:P:341:PRO:HD3	2:P:399:VAL:HG11	1.96	0.47
1:E:83:SER:O	1:E:86:PHE:HB3	2.13	0.47
2:G:532:SER:O	2:G:536:ILE:HG13	2.13	0.47
2:H:436:TRP:HB3	2:H:494:LEU:HD11	1.96	0.47
2:O:313:TYR:CZ	2:O:315:SER:HA	2.49	0.47
2:C:297:LEU:N	2:C:298:PRO:CD	2.78	0.47
2:P:139:ASN:OD1	2:P:141:ALA:HB3	2.14	0.47
2:P:378:ASP:CB	2:P:379:PRO:HD3	2.45	0.47
2:C:225:ASN:HB2	2:C:369:TRP:CE2	2.49	0.47
2:G:241:SER:O	2:G:366:PHE:HA	2.14	0.47
2:G:562:VAL:HG11	10:G:939:HOH:O	2.12	0.47
2:P:333:ARG:HH11	2:P:421:ASN:HD22	1.62	0.47
2:G:116:GLU:HG2	10:G:779:HOH:O	2.13	0.47
1:I:16:ASN:O	1:I:20:PRO:HA	2.14	0.47
2:O:549:ASN:ND2	10:O:702:HOH:O	2.40	0.47
2:D:211:LEU:HD23	2:D:254:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:ILE:HD13	2:H:464:LEU:CD2	2.44	0.47
2:H:576:ARG:HG2	2:H:578:ALA:HB2	1.96	0.47
2:L:333:ARG:HH11	2:L:421:ASN:HD22	1.62	0.47
2:O:242:GLU:HG3	6:O:605:0KY:O2	2.15	0.47
2:G:259:ARG:O	2:G:263:GLU:HG3	2.15	0.47
2:K:349:ARG:HB2	2:K:351:GLN:HG2	1.97	0.47
2:O:215:ASN:HB3	10:O:863:HOH:O	2.13	0.47
2:H:559:ARG:HB2	10:H:819:HOH:O	2.15	0.46
2:O:370:ARG:HG2	2:O:374:GLU:OE2	2.15	0.46
1:B:64:VAL:HG13	1:B:68:ILE:HD12	1.97	0.46
2:D:223:LEU:HA	2:D:226:ARG:NE	2.30	0.46
1:E:5:ASP:OD1	1:E:5:ASP:N	2.47	0.46
2:G:199:VAL:HG12	2:G:254:LEU:HD21	1.96	0.46
2:H:241:SER:O	2:H:366:PHE:HA	2.15	0.46
2:L:466:GLU:HB2	10:L:936:HOH:O	2.15	0.46
2:D:305:ALA:HB2	2:D:486:LYS:HZ2	1.80	0.46
7:L:601:HEM:HBC2	7:L:601:HEM:CMC	2.42	0.46
2:L:265:LYS:HD2	2:L:269:PRO:HA	1.97	0.46
2:P:297:LEU:N	2:P:298:PRO:CD	2.79	0.46
2:P:361:LEU:O	2:P:364:VAL:HG22	2.16	0.46
2:C:504:ARG:HD3	3:Q:6:FUC:H62	1.98	0.46
1:B:79:ASP:O	2:D:388:PRO:HB3	2.16	0.46
2:G:297:LEU:N	2:G:298:PRO:CD	2.79	0.46
1:I:83:SER:HB3	2:K:554:SER:O	2.16	0.46
2:L:132:PRO:O	2:L:133:ASN:HB2	2.16	0.46
2:G:531:ILE:HD12	2:G:531:ILE:O	2.15	0.46
2:L:213:PHE:CG	2:L:231:PRO:HG2	2.51	0.46
2:P:335:GLY:HA3	7:P:601:HEM:CBC	2.46	0.46
2:P:349:ARG:HG3	2:P:351:GLN:HG2	1.98	0.46
2:C:128:LEU:HD12	2:C:128:LEU:N	2.31	0.45
2:H:359:VAL:HG12	2:H:364:VAL:CG1	2.46	0.45
1:M:13:MET:O	1:M:14:CYS:HB2	2.16	0.45
2:C:307:ARG:HD3	10:C:986:HOH:O	2.15	0.45
1:B:63:ALA:O	1:B:67:GLU:HG2	2.16	0.45
7:D:601:HEM:CAA	6:D:602:0KY:S	3.05	0.45
2:G:271:TRP:CZ3	2:G:279:GLU:HG3	2.51	0.45
1:F:41:PHE:CD1	1:F:42:SER:HB2	2.52	0.45
7:H:601:HEM:HAA2	6:H:605:0KY:S	2.56	0.45
2:K:213:PHE:CG	2:K:231:PRO:HG2	2.52	0.45
1:J:98:ASP:OD2	7:L:601:HEM:O1D	2.34	0.45
1:M:11:THR:O	1:M:24:ALA:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLY:HA2	1:B:20:PRO:HD2	1.99	0.45
2:G:267:LEU:HD22	2:G:576:ARG:NH2	2.31	0.45
7:G:601:HEM:HBA1	6:G:605:0KY:S	2.55	0.45
2:O:533:LEU:HD23	2:O:551:ILE:HD13	1.98	0.45
1:B:32:TRP:CE2	2:D:325:ALA:HB2	2.52	0.45
2:G:171:VAL:HG12	2:G:288:VAL:HG12	1.99	0.45
2:K:377:ILE:HD12	2:K:381:LEU:HD11	1.98	0.45
1:J:41:PHE:CD1	1:J:42:SER:HB2	2.51	0.45
1:F:70:ARG:NH1	2:H:403:ARG:HH21	2.15	0.45
2:L:333:ARG:HH11	2:L:421:ASN:ND2	2.15	0.45
2:C:533:LEU:N	2:C:534:PRO:HD2	2.32	0.45
2:O:336:HIS:CE1	2:O:417:LEU:HD11	2.51	0.45
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.99	0.45
2:G:208:ARG:NE	10:G:701:HOH:O	2.48	0.45
2:P:411:MET:SD	2:P:415:LEU:HD11	2.57	0.45
2:C:406:LEU:HD22	2:C:417:LEU:HB2	1.98	0.44
2:K:241:SER:O	2:K:366:PHE:HA	2.17	0.44
2:K:333:ARG:HH11	2:K:421:ASN:ND2	2.14	0.44
2:L:241:SER:O	2:L:366:PHE:HA	2.18	0.44
2:D:213:PHE:CG	2:D:231:PRO:HG2	2.52	0.44
1:E:88:GLN:OE1	2:G:245:GLU:HB2	2.17	0.44
2:G:157:ASN:OD1	2:G:158:ILE:HG13	2.18	0.44
1:I:32:TRP:CE2	2:K:325:ALA:HB2	2.52	0.44
2:K:275:ARG:CD	10:K:758:HOH:O	2.64	0.44
2:K:406:LEU:HD22	2:K:417:LEU:HB2	1.98	0.44
7:K:601:HEM:HAA2	6:K:602:0KY:S	2.58	0.44
2:K:354:GLU:HA	2:K:354:GLU:OE1	2.17	0.44
2:P:181:GLU:N	2:P:182:PRO:CD	2.81	0.44
2:C:336:HIS:CE1	2:C:417:LEU:HD21	2.53	0.44
2:H:301:LEU:HB3	2:H:305:ALA:CB	2.46	0.44
2:K:308:LYS:HD3	2:K:309:TYR:CZ	2.52	0.44
2:O:200:ASN:HD22	2:O:203:PHE:N	2.06	0.44
2:O:406:LEU:HD23	2:O:415:LEU:HB2	1.99	0.44
2:C:241:SER:O	2:C:366:PHE:HA	2.17	0.44
2:H:175:MET:HG3	2:H:176:VAL:HG23	1.99	0.44
2:C:333:ARG:HD3	2:C:421:ASN:ND2	2.32	0.44
2:G:172:ASP:O	2:G:173:ALA:HB3	2.18	0.44
1:F:13:MET:O	1:F:14:CYS:HB2	2.18	0.44
2:K:197:LEU:HB2	2:K:254:LEU:HD12	2.00	0.44
1:N:64:VAL:CG1	1:N:68:ILE:HD12	2.41	0.44
2:P:173:ALA:HA	2:P:175:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:362:SER:HA	2:C:365:PHE:CE1	2.52	0.44
2:O:465:MET:CE	2:O:471:PRO:HD3	2.47	0.44
2:P:523:GLN:HG2	10:P:902:HOH:O	2.18	0.44
6:C:601:0KY:S	7:C:602:HEM:HAA2	2.58	0.43
1:E:31:ARG:CZ	1:E:35:ALA:HB2	2.48	0.43
2:K:570:LEU:HD23	2:K:572:LEU:HD21	1.99	0.43
2:L:199:VAL:HG12	2:L:254:LEU:HD21	2.00	0.43
2:L:270:ARG:HD3	10:L:814:HOH:O	2.17	0.43
1:B:56:PHE:CD1	2:D:469:GLY:HA3	2.52	0.43
2:G:299:LEU:N	2:G:299:LEU:CD1	2.81	0.43
1:F:68:ILE:CD1	2:H:464:LEU:HD23	2.47	0.43
2:O:571:ASN:HA	10:O:820:HOH:O	2.17	0.43
2:H:456:ARG:NH2	10:H:720:HOH:O	2.52	0.43
2:C:128:LEU:HB2	2:C:144:ILE:HB	2.01	0.43
2:C:304:THR:HG21	10:C:902:HOH:O	2.18	0.43
2:G:181:GLU:HB2	10:G:850:HOH:O	2.17	0.43
2:C:242:GLU:O	2:C:365:PHE:HA	2.18	0.43
2:K:554:SER:HB3	2:K:560:ASP:HB3	2.00	0.43
2:P:354:GLU:HB3	2:P:355:PRO:HA	2.00	0.43
1:F:96:ASP:OD2	2:H:175:MET:CE	2.65	0.43
2:H:390:LYS:NZ	2:H:396:GLN:O	2.37	0.43
2:K:569:ALA:O	2:K:570:LEU:C	2.56	0.43
7:L:601:HEM:HAA2	6:L:602:0KY:S	2.59	0.43
2:O:465:MET:HE1	2:O:469:GLY:O	2.19	0.43
7:D:601:HEM:CBA	6:D:602:0KY:S	3.03	0.43
2:K:377:ILE:O	2:K:381:LEU:HG	2.19	0.43
2:L:181:GLU:OE2	2:L:184:ALA:HB3	2.18	0.43
2:L:378:ASP:HB2	2:L:379:PRO:HD3	2.00	0.43
2:G:533:LEU:N	2:G:534:PRO:CD	2.82	0.43
2:P:309:TYR:CZ	2:P:497:CYS:HA	2.54	0.43
2:G:504:ARG:HB3	10:G:884:HOH:O	2.19	0.43
2:G:567:LEU:HA	2:G:568:PRO:HD3	1.91	0.43
2:K:158:ILE:HD13	2:L:164:ILE:HD13	2.01	0.43
2:K:299:LEU:CD2	2:K:552:PHE:HB2	2.49	0.43
2:O:535:ARG:NH2	2:O:539:ASP:OD2	2.50	0.43
2:O:559:ARG:HD2	10:O:862:HOH:O	2.18	0.43
1:B:29:PHE:CZ	2:D:329:THR:HG21	2.53	0.42
6:D:602:0KY:H11	6:D:602:0KY:C6	2.49	0.42
2:L:514:TRP:CE2	2:L:515:GLU:HG3	2.54	0.42
1:M:59:ALA:HB2	2:O:467:GLN:O	2.18	0.42
1:E:13:MET:O	1:E:14:CYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:347:ASP:CB	1:I:80:GLN:OE1	2.54	0.42
2:G:242:GLU:OE1	7:G:601:HEM:HBB2	2.18	0.42
2:H:353:MET:HE2	10:H:711:HOH:O	2.18	0.42
2:G:225:ASN:C	2:G:225:ASN:OD1	2.58	0.42
2:G:369:TRP:CZ3	8:G:603:NAG:H2	2.54	0.42
2:H:271:TRP:CZ3	2:H:279:GLU:HG3	2.55	0.42
2:H:491:VAL:HB	2:H:495:LEU:HB2	2.01	0.42
2:H:530:GLN:HG3	10:H:740:HOH:O	2.19	0.42
2:D:122:GLN:O	2:D:123:PRO:C	2.56	0.42
2:G:304:THR:HG23	10:G:761:HOH:O	2.19	0.42
1:F:83:SER:HB3	2:H:554:SER:O	2.20	0.42
2:H:139:ASN:OD1	2:H:141:ALA:HB3	2.19	0.42
2:L:228:ALA:HB3	10:L:759:HOH:O	2.19	0.42
2:O:212:PRO:HB3	10:O:768:HOH:O	2.19	0.42
2:O:318:ASP:OD1	2:O:318:ASP:C	2.57	0.42
1:B:6:LYS:HZ2	2:D:275:ARG:NH2	2.13	0.42
1:B:29:PHE:CE1	2:D:165:ASN:HB2	2.55	0.42
2:G:314:ARG:HA	2:G:314:ARG:HD3	1.86	0.42
2:H:411:MET:HE2	2:H:415:LEU:CD2	2.48	0.42
2:K:297:LEU:N	2:K:298:PRO:CD	2.83	0.42
2:K:465:MET:HE3	2:K:469:GLY:O	2.19	0.42
2:O:304:THR:CG2	10:O:861:HOH:O	2.59	0.42
2:D:486:LYS:NZ	10:D:720:HOH:O	2.53	0.42
2:K:558:PRO:O	2:K:559:ARG:C	2.58	0.42
2:D:549:ASN:HB3	10:D:760:HOH:O	2.20	0.42
2:G:565:SER:C	2:G:567:LEU:H	2.23	0.42
2:K:181:GLU:HB2	10:K:779:HOH:O	2.20	0.42
2:K:309:TYR:CZ	2:K:497:CYS:HA	2.55	0.42
2:O:462:ARG:HB3	10:O:704:HOH:O	2.20	0.42
2:O:535:ARG:HA	2:O:535:ARG:HD2	1.93	0.42
2:O:308:LYS:NZ	3:X:4:MAN:O6	2.49	0.42
2:O:378:ASP:OD1	2:O:541:THR:HB	2.20	0.42
2:C:309:TYR:OH	2:C:497:CYS:HB2	2.19	0.41
2:D:304:THR:HG22	10:D:720:HOH:O	2.20	0.41
1:B:69:VAL:CG1	2:D:398:ALA:HB3	2.50	0.41
2:D:393:ARG:CD	10:D:789:HOH:O	2.68	0.41
2:G:465:MET:HE3	10:G:823:HOH:O	2.20	0.41
2:H:471:PRO:HA	2:H:474:ILE:HG13	2.02	0.41
2:L:522:MET:O	2:L:526:GLN:HG3	2.20	0.41
2:O:279:GLU:O	2:O:283:ILE:HG13	2.19	0.41
2:L:308:LYS:HD3	2:L:309:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:29:PHE:CE1	2:O:165:ASN:HB2	2.55	0.41
1:E:82:ARG:HA	2:G:552:PHE:O	2.20	0.41
2:C:521:SER:OG	2:C:524:GLN:HG3	2.19	0.41
2:D:113:VAL:HG21	2:D:122:GLN:HB2	2.01	0.41
1:I:4:GLN:HA	1:I:17:ARG:HH12	1.85	0.41
1:N:53:ARG:O	1:N:54:ASN:C	2.59	0.41
2:P:187:LEU:HD11	2:P:236:GLY:HA2	2.02	0.41
1:A:20:PRO:HD2	1:B:40:GLY:HA2	2.03	0.41
2:G:335:GLY:HA3	7:G:601:HEM:HBC2	2.03	0.41
2:L:354:GLU:HB3	2:L:355:PRO:HA	2.01	0.41
2:L:417:LEU:HB3	2:L:418:PRO:HD3	2.03	0.41
2:P:181:GLU:OE1	2:P:185:ARG:NH1	2.54	0.41
2:P:223:LEU:HD22	2:P:226:ARG:HH12	1.85	0.41
2:C:113:VAL:O	10:C:701:HOH:O	2.22	0.41
2:L:242:GLU:O	2:L:365:PHE:HA	2.20	0.41
1:M:10:ILE:HD13	1:M:10:ILE:HA	1.86	0.41
2:O:491:VAL:HB	2:O:495:LEU:HB2	2.03	0.41
2:P:113:VAL:CG1	2:P:125:CYS:SG	3.08	0.41
2:P:378:ASP:OD1	2:P:541:THR:HB	2.21	0.41
2:C:514:TRP:CE2	2:C:515:GLU:HG3	2.56	0.41
1:B:13:MET:O	1:B:14:CYS:HB2	2.21	0.41
2:G:282:LYS:HG2	2:G:520:PHE:CZ	2.56	0.41
1:F:38:GLU:CD	1:F:48:THR:HG1	2.14	0.41
2:H:175:MET:HE1	2:H:288:VAL:CG2	2.49	0.41
2:H:214:ASP:OD1	2:H:215:ASN:N	2.53	0.41
2:K:345:ARG:O	2:K:346:LEU:HD23	2.21	0.41
2:L:393:ARG:HB2	2:L:396:GLN:HB2	2.02	0.41
2:O:257:HIS:CE1	2:O:280:ALA:HB3	2.56	0.41
2:O:548:LYS:HZ3	2:O:562:VAL:HG12	1.84	0.41
2:P:181:GLU:CG	10:P:726:HOH:O	2.62	0.41
2:P:182:PRO:HG2	10:P:890:HOH:O	2.19	0.41
2:P:182:PRO:HG3	10:P:890:HOH:O	2.19	0.41
2:P:445:PRO:O	2:P:471:PRO:HG2	2.21	0.41
2:D:362:SER:HA	2:D:365:PHE:CE1	2.56	0.41
2:D:411:MET:HE1	2:D:415:LEU:HD21	2.03	0.41
2:G:346:LEU:HD23	2:G:346:LEU:HA	1.92	0.41
1:I:84:LEU:HD12	1:I:84:LEU:HA	1.94	0.41
2:O:305:ALA:HB2	2:O:486:LYS:HE3	2.02	0.41
1:E:32:TRP:CE2	2:G:325:ALA:HB2	2.56	0.40
2:G:339:ILE:HG23	10:G:841:HOH:O	2.20	0.40
2:L:181:GLU:HG3	2:L:185:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:173:ALA:HA	2:O:175:MET:SD	2.62	0.40
2:G:535:ARG:O	2:G:538:CYS:HB2	2.21	0.40
2:H:476:ILE:HG23	2:H:477:TRP:N	2.35	0.40
7:H:601:HEM:HMC2	7:H:601:HEM:CBC	2.41	0.40
2:K:252:LEU:HD11	2:K:537:ILE:HA	2.02	0.40
1:N:100:THR:HG21	2:P:428:HIS:CE1	2.55	0.40
2:D:458:LEU:O	2:D:462:ARG:HG3	2.21	0.40
2:D:563:ASN:HB3	10:D:877:HOH:O	2.20	0.40
2:K:533:LEU:HB3	2:K:534:PRO:HD3	2.03	0.40
2:L:145:PRO:HG2	2:L:411:MET:HE1	2.02	0.40
2:C:207:GLY:N	10:C:712:HOH:O	2.46	0.40
2:D:297:LEU:N	2:D:298:PRO:CD	2.85	0.40
2:D:373:LEU:HD13	8:D:604:NAG:H61	2.04	0.40
2:G:347:ASP:C	2:G:347:ASP:OD1	2.58	0.40
1:F:64:VAL:HG13	1:F:68:ILE:CD1	2.45	0.40
2:P:134:ASP:CG	2:P:135:PRO:HD2	2.42	0.40
2:D:216:LEU:HD23	2:D:216:LEU:HA	1.95	0.40
1:F:80:GLN:HB2	1:F:81:GLU:OE2	2.21	0.40
2:H:304:THR:HG22	10:H:893:HOH:O	2.22	0.40
2:H:400:ASP:O	2:H:404:GLU:HB2	2.22	0.40
2:K:517:GLU:HA	2:K:517:GLU:OE1	2.22	0.40
2:O:219:ASP:HB3	2:O:222:LEU:HD12	2.03	0.40
2:O:297:LEU:N	2:O:298:PRO:HD2	2.36	0.40
2:P:533:LEU:N	2:P:534:PRO:CD	2.85	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)
2:G:522:MET:SD	10:L:923:HOH:O[1_556]	2.14	0.06

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	102/104 (98%)	101 (99%)	1 (1%)	0	100	100
1	B	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
1	E	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
1	F	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
1	I	102/104 (98%)	97 (95%)	4 (4%)	1 (1%)	13	8
1	J	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
1	M	102/104 (98%)	98 (96%)	2 (2%)	2 (2%)	6	2
1	N	103/104 (99%)	100 (97%)	3 (3%)	0	100	100
2	C	463/466 (99%)	449 (97%)	14 (3%)	0	100	100
2	D	463/466 (99%)	443 (96%)	19 (4%)	1 (0%)	44	42
2	G	462/466 (99%)	440 (95%)	19 (4%)	3 (1%)	22	17
2	H	463/466 (99%)	442 (96%)	21 (4%)	0	100	100
2	K	462/466 (99%)	438 (95%)	23 (5%)	1 (0%)	44	42
2	L	463/466 (99%)	447 (96%)	16 (4%)	0	100	100
2	O	463/466 (99%)	442 (96%)	19 (4%)	2 (0%)	30	27
2	P	463/466 (99%)	447 (96%)	16 (4%)	0	100	100
All	All	4519/4560 (99%)	4337 (96%)	172 (4%)	10 (0%)	44	42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	114	ASN
2	G	142	ASP
1	I	3	GLU
2	K	114	ASN
1	M	3	GLU
2	D	217	HIS
2	G	217	HIS
2	O	142	ASP
1	M	2	PRO
2	O	217	HIS

5.3.2 Protein sidechains (i)

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	90/90 (100%)	90 (100%)	0	100	100
1	B	90/90 (100%)	89 (99%)	1 (1%)	70	76
1	E	90/90 (100%)	89 (99%)	1 (1%)	70	76
1	F	90/90 (100%)	87 (97%)	3 (3%)	33	33
1	I	90/90 (100%)	88 (98%)	2 (2%)	47	51
1	J	90/90 (100%)	89 (99%)	1 (1%)	70	76
1	M	90/90 (100%)	89 (99%)	1 (1%)	70	76
1	N	91/90 (101%)	88 (97%)	3 (3%)	33	33
2	C	410/410 (100%)	405 (99%)	5 (1%)	67	73
2	D	409/410 (100%)	395 (97%)	14 (3%)	32	32
2	G	410/410 (100%)	398 (97%)	12 (3%)	37	39
2	H	409/410 (100%)	405 (99%)	4 (1%)	73	78
2	K	410/410 (100%)	401 (98%)	9 (2%)	47	51
2	L	409/410 (100%)	402 (98%)	7 (2%)	56	61
2	O	409/410 (100%)	399 (98%)	10 (2%)	44	47
2	P	410/410 (100%)	403 (98%)	7 (2%)	56	61
All	All	3997/4000 (100%)	3917 (98%)	80 (2%)	50	55

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	118	SER
2	C	175	MET
2	C	444	GLN
2	C	504	ARG
2	C	576	ARG
1	B	75	GLN
2	D	175	MET
2	D	217	HIS

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Mol	Chain	Res	Type
2	D	219	ASP
2	D	227	SER
2	D	254	LEU
2	D	334	TYR
2	D	349	ARG
2	D	358	ARG
2	D	363	ARG
2	D	466	GLU
2	D	470	THR
2	D	497	CYS
2	D	522	MET
2	D	553	MET
1	E	42	SER
2	G	142	ASP
2	G	175	MET
2	G	227	SER
2	G	243	MET
2	G	267	LEU
2	G	330	ASN
2	G	353	MET
2	G	526	GLN
2	G	546	VAL
2	G	547	SER
2	G	563	ASN
2	G	576	ARG
1	F	6	LYS
1	F	60	LEU
1	F	84	LEU
2	H	265	LYS
2	H	466	GLU
2	H	526	GLN
2	H	576	ARG
1	I	5	ASP
1	I	52	LYS
2	K	113	VAL
2	K	175	MET
2	K	181	GLU
2	K	214	ASP
2	K	304	THR
2	K	314	ARG
2	K	318	ASP
2	K	358	ARG

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Mol	Chain	Res	Type
2	K	565	SER
1	J	42	SER
2	L	175	MET
2	L	180	GLU
2	L	215	ASN
2	L	254	LEU
2	L	408	GLU
2	L	470	THR
2	L	486	LYS
1	M	80	GLN
2	O	116	GLU
2	O	175	MET
2	O	180	GLU
2	O	229	ARG
2	O	304	THR
2	O	330	ASN
2	O	408	GLU
2	O	466	GLU
2	O	497	CYS
2	O	547	SER
1	N	60	LEU
1	N	75	GLN
1	N	81	GLU
2	P	175	MET
2	P	181	GLU
2	P	254	LEU
2	P	318	ASP
2	P	349	ARG
2	P	470	THR
2	P	547	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	121	GLN
2	C	133	ASN
2	C	348	ASN
2	C	421	ASN
2	D	140	GLN
2	D	201	GLN
2	D	421	ASN
2	D	467	GLN

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Mol	Chain	Res	Type
2	D	549	ASN
1	E	26	ASN
2	G	121	GLN
2	G	206	ASN
2	G	351	GLN
2	G	421	ASN
2	G	549	ASN
1	F	26	ASN
2	H	140	GLN
2	H	157	ASN
2	H	201	GLN
2	H	563	ASN
1	I	16	ASN
2	K	133	ASN
2	K	201	GLN
2	K	421	ASN
2	K	530	GLN
2	K	549	ASN
2	L	121	GLN
2	L	193	GLN
2	L	201	GLN
2	L	215	ASN
2	L	217	HIS
2	L	421	ASN
1	M	16	ASN
2	O	140	GLN
2	O	200	ASN
2	O	217	HIS
2	O	356	ASN
2	O	421	ASN
2	O	549	ASN
1	N	26	ASN
2	P	193	GLN
2	P	217	HIS
2	P	421	ASN
2	P	467	GLN
2	P	549	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	CSO	O	150	2	3,6,7	0.46	0	1,6,8	0.57	0
2	CSO	P	150	2	3,6,7	0.72	0	1,6,8	0.58	0
2	CSO	C	150	2	3,6,7	0.76	0	1,6,8	0.95	0
2	CSO	D	150	2	3,6,7	0.62	0	1,6,8	1.29	0
2	CSO	H	150	2	3,6,7	0.59	0	1,6,8	1.48	0
2	CSO	K	150	2	3,6,7	0.60	0	1,6,8	1.86	0
2	CSO	L	150	2	3,6,7	0.58	0	1,6,8	1.00	0
2	CSO	G	150	2	3,6,7	0.79	0	1,6,8	1.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	O	150	2	-	0/1/5/7	-
2	CSO	P	150	2	-	0/1/5/7	-
2	CSO	C	150	2	-	0/1/5/7	-
2	CSO	D	150	2	-	0/1/5/7	-
2	CSO	H	150	2	-	0/1/5/7	-
2	CSO	K	150	2	-	0/1/5/7	-
2	CSO	L	150	2	-	0/1/5/7	-
2	CSO	G	150	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

53 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	$\#\|Z\| > 2$
3	NAG	Q	1	3,2	14,14,15	0.48	0	17,19,21	1.73	3 (17%)
3	NAG	Q	2	3	14,14,15	0.69	0	17,19,21	1.03	1 (5%)
3	BMA	Q	3	3	11,11,12	0.46	0	15,15,17	0.87	1 (6%)
3	MAN	Q	4	3	11,11,12	0.66	0	15,15,17	0.90	0
3	MAN	Q	5	3	11,11,12	0.75	0	15,15,17	0.89	0
3	FUC	Q	6	3	10,10,11	0.86	0	14,14,16	1.30	1 (7%)
3	NAG	R	1	3,2	14,14,15	0.65	0	17,19,21	1.45	2 (11%)
3	NAG	R	2	3	14,14,15	0.75	0	17,19,21	0.80	0
3	BMA	R	3	3	11,11,12	0.53	0	15,15,17	1.34	3 (20%)
3	MAN	R	4	3	11,11,12	0.60	0	15,15,17	0.83	0
3	MAN	R	5	3	11,11,12	0.54	0	15,15,17	1.10	2 (13%)
3	FUC	R	6	3	10,10,11	0.73	0	14,14,16	1.35	1 (7%)
3	NAG	S	1	3,2	14,14,15	0.55	0	17,19,21	1.82	4 (23%)
3	NAG	S	2	3	14,14,15	0.55	0	17,19,21	1.04	1 (5%)
3	BMA	S	3	3	11,11,12	0.40	0	15,15,17	1.07	1 (6%)
3	MAN	S	4	3	11,11,12	0.61	0	15,15,17	0.82	0
3	MAN	S	5	3	11,11,12	0.44	0	15,15,17	0.89	0
3	FUC	S	6	3	10,10,11	0.82	1 (10%)	14,14,16	1.22	2 (14%)
3	NAG	T	1	3,2	14,14,15	0.49	0	17,19,21	1.32	1 (5%)
3	NAG	T	2	3	14,14,15	0.59	0	17,19,21	0.87	0
3	BMA	T	3	3	11,11,12	0.39	0	15,15,17	0.68	0
3	MAN	T	4	3	11,11,12	0.65	0	15,15,17	0.89	1 (6%)
3	MAN	T	5	3	11,11,12	0.67	0	15,15,17	0.98	1 (6%)
3	FUC	T	6	3	10,10,11	1.03	1 (10%)	14,14,16	1.32	3 (21%)
3	NAG	U	1	3,2	14,14,15	0.56	0	17,19,21	1.52	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	U	2	3	14,14,15	0.88	1 (7%)	17,19,21	1.14	1 (5%)
3	BMA	U	3	3	11,11,12	0.56	0	15,15,17	1.03	0
3	MAN	U	4	3	11,11,12	0.51	0	15,15,17	0.67	0
3	MAN	U	5	3	11,11,12	0.61	0	15,15,17	0.99	0
3	FUC	U	6	3	10,10,11	0.69	0	14,14,16	1.30	2 (14%)
3	NAG	V	1	3,2	14,14,15	0.47	0	17,19,21	1.53	3 (17%)
3	NAG	V	2	3	14,14,15	0.78	0	17,19,21	1.23	1 (5%)
3	BMA	V	3	3	11,11,12	0.45	0	15,15,17	1.09	1 (6%)
3	MAN	V	4	3	11,11,12	0.62	0	15,15,17	1.18	2 (13%)
3	MAN	V	5	3	11,11,12	0.45	0	15,15,17	1.05	1 (6%)
3	FUC	V	6	3	10,10,11	0.79	0	14,14,16	1.04	1 (7%)
3	NAG	W	1	3,2	14,14,15	0.61	0	17,19,21	1.73	2 (11%)
3	NAG	W	2	3	14,14,15	0.77	1 (7%)	17,19,21	1.25	2 (11%)
3	BMA	W	3	3	11,11,12	0.48	0	15,15,17	1.02	1 (6%)
3	MAN	W	4	3	11,11,12	0.70	0	15,15,17	0.63	0
3	MAN	W	5	3	11,11,12	0.62	0	15,15,17	0.69	0
3	FUC	W	6	3	10,10,11	0.74	0	14,14,16	1.34	2 (14%)
3	NAG	X	1	3,2	14,14,15	0.51	0	17,19,21	1.60	4 (23%)
3	NAG	X	2	3	14,14,15	0.60	0	17,19,21	0.86	1 (5%)
3	BMA	X	3	3	11,11,12	0.36	0	15,15,17	1.17	1 (6%)
3	MAN	X	4	3	11,11,12	0.54	0	15,15,17	1.23	3 (20%)
3	MAN	X	5	3	11,11,12	0.59	0	15,15,17	0.96	1 (6%)
3	FUC	X	6	3	10,10,11	1.05	1 (10%)	14,14,16	0.89	0
4	NAG	Y	1	4,2	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
4	NAG	Y	2	4	14,14,15	0.74	0	17,19,21	0.89	0
4	BMA	Y	3	4	11,11,12	0.27	0	15,15,17	0.83	0
4	MAN	Y	4	4	11,11,12	0.48	0	15,15,17	0.98	1 (6%)
4	MAN	Y	5	4	11,11,12	0.63	0	15,15,17	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	Q	4	3	-	0/2/19/22	0/1/1/1
3	MAN	Q	5	3	-	0/2/19/22	0/1/1/1
3	FUC	Q	6	3	-	-	0/1/1/1
3	NAG	R	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	BMA	R	3	3	-	0/2/19/22	0/1/1/1
3	MAN	R	4	3	-	2/2/19/22	0/1/1/1
3	MAN	R	5	3	-	0/2/19/22	0/1/1/1
3	FUC	R	6	3	-	-	0/1/1/1
3	NAG	S	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	BMA	S	3	3	-	0/2/19/22	0/1/1/1
3	MAN	S	4	3	-	2/2/19/22	0/1/1/1
3	MAN	S	5	3	-	1/2/19/22	0/1/1/1
3	FUC	S	6	3	-	-	0/1/1/1
3	NAG	T	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	1/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
3	MAN	T	4	3	-	2/2/19/22	0/1/1/1
3	MAN	T	5	3	-	0/2/19/22	0/1/1/1
3	FUC	T	6	3	-	-	0/1/1/1
3	NAG	U	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1
3	MAN	U	4	3	-	2/2/19/22	0/1/1/1
3	MAN	U	5	3	-	2/2/19/22	0/1/1/1
3	FUC	U	6	3	-	-	0/1/1/1
3	NAG	V	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1
3	MAN	V	4	3	-	2/2/19/22	0/1/1/1
3	MAN	V	5	3	-	0/2/19/22	0/1/1/1
3	FUC	V	6	3	-	-	0/1/1/1
3	NAG	W	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	BMA	W	3	3	-	0/2/19/22	0/1/1/1
3	MAN	W	4	3	-	2/2/19/22	0/1/1/1
3	MAN	W	5	3	-	0/2/19/22	0/1/1/1
3	FUC	W	6	3	-	-	0/1/1/1
3	NAG	X	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	X	3	3	-	0/2/19/22	0/1/1/1
3	MAN	X	4	3	-	0/2/19/22	0/1/1/1
3	MAN	X	5	3	-	0/2/19/22	0/1/1/1
3	FUC	X	6	3	-	-	0/1/1/1
4	NAG	Y	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Y	3	4	-	0/2/19/22	0/1/1/1
4	MAN	Y	4	4	-	2/2/19/22	0/1/1/1
4	MAN	Y	5	4	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	6	FUC	O5-C1	-2.54	1.39	1.43
3	T	6	FUC	O5-C1	-2.52	1.39	1.43
3	W	2	NAG	C1-C2	2.33	1.55	1.52
3	U	2	NAG	O5-C1	-2.14	1.40	1.43
3	S	6	FUC	O5-C1	-2.05	1.40	1.43

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	W	1	NAG	C1-O5-C5	6.02	120.25	112.19
3	U	1	NAG	O5-C1-C2	-5.40	102.94	111.29
3	Q	1	NAG	O5-C1-C2	-4.77	103.91	111.29
3	Q	1	NAG	C1-O5-C5	3.99	117.54	112.19
3	S	1	NAG	C1-O5-C5	3.94	117.47	112.19
3	S	1	NAG	O5-C1-C2	-3.92	105.22	111.29
3	V	1	NAG	O5-C1-C2	-3.88	105.29	111.29
3	T	1	NAG	O5-C1-C2	-3.68	105.60	111.29
3	Q	6	FUC	C1-C2-C3	-3.42	104.66	109.64
3	R	1	NAG	C1-O5-C5	3.41	116.75	112.19
3	R	6	FUC	C6-C5-C4	-3.33	106.98	113.08
3	X	1	NAG	O5-C1-C2	-3.26	106.25	111.29
3	S	6	FUC	C1-C2-C3	-3.25	104.91	109.64
3	R	1	NAG	O5-C1-C2	-3.17	106.39	111.29
3	W	6	FUC	C1-C2-C3	-3.16	105.05	109.64
4	Y	4	MAN	C1-O5-C5	3.15	116.40	112.19
3	V	5	MAN	O5-C5-C6	3.12	113.74	107.66
3	S	2	NAG	C4-C3-C2	-3.03	106.57	111.02
3	X	1	NAG	C1-O5-C5	3.03	116.24	112.19
3	X	3	BMA	C1-C2-C3	2.98	113.99	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	5	MAN	C1-O5-C5	2.98	116.17	112.19
3	S	3	BMA	C1-C2-C3	2.96	113.96	109.64
3	X	1	NAG	C1-C2-N2	2.82	114.88	110.43
3	R	3	BMA	O3-C3-C2	-2.79	104.36	110.05
3	R	3	BMA	O2-C2-C3	-2.74	104.48	110.15
3	W	3	BMA	C1-C2-C3	2.70	113.57	109.64
3	W	2	NAG	O3-C3-C2	2.70	115.00	109.40
3	T	6	FUC	C6-C5-C4	-2.65	108.23	113.08
3	T	4	MAN	C1-O5-C5	2.62	115.70	112.19
3	R	5	MAN	O5-C5-C6	2.57	112.67	107.66
3	V	2	NAG	O5-C1-C2	-2.49	107.44	111.29
3	V	4	MAN	C2-C3-C4	-2.48	106.50	110.86
3	R	3	BMA	C1-C2-C3	2.43	113.18	109.64
3	T	5	MAN	C1-O5-C5	2.41	115.42	112.19
3	V	6	FUC	O5-C5-C4	2.38	113.84	109.55
3	W	2	NAG	C4-C3-C2	-2.35	107.57	111.02
3	V	3	BMA	O5-C5-C6	2.34	112.22	107.66
3	W	1	NAG	O4-C4-C3	-2.32	104.91	110.38
3	T	6	FUC	C1-C2-C3	-2.31	106.28	109.64
3	X	4	MAN	C1-O5-C5	2.30	115.26	112.19
4	Y	1	NAG	C1-C2-N2	2.29	114.04	110.43
3	X	4	MAN	C6-C5-C4	-2.27	107.44	113.02
3	X	4	MAN	C3-C4-C5	2.26	114.33	110.23
3	V	4	MAN	C1-O5-C5	2.25	115.20	112.19
3	S	1	NAG	O4-C4-C3	-2.20	105.18	110.38
3	V	1	NAG	C6-C5-C4	-2.20	107.63	113.02
3	S	6	FUC	O5-C5-C6	2.18	112.14	107.40
3	U	6	FUC	C1-C2-C3	-2.17	106.48	109.64
3	U	6	FUC	C3-C4-C5	2.14	113.06	109.81
3	X	2	NAG	O7-C7-C8	-2.13	118.25	122.05
3	Q	1	NAG	C1-C2-N2	2.13	113.79	110.43
3	R	5	MAN	C1-O5-C5	2.12	115.03	112.19
3	V	1	NAG	O4-C4-C3	-2.12	105.39	110.38
3	W	6	FUC	C6-C5-C4	-2.11	109.22	113.08
3	S	1	NAG	O3-C3-C2	2.11	113.78	109.40
3	Q	2	NAG	C1-C2-N2	-2.08	107.15	110.43
3	T	6	FUC	C3-C4-C5	2.08	112.98	109.81
3	U	2	NAG	C1-C2-N2	-2.06	107.19	110.43
3	Q	3	BMA	C1-C2-C3	2.05	112.64	109.64
3	X	1	NAG	O4-C4-C3	-2.03	105.60	110.38

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	5	MAN	C4-C5-C6-O6
3	S	4	MAN	O5-C5-C6-O6
3	W	4	MAN	O5-C5-C6-O6
4	Y	5	MAN	O5-C5-C6-O6
3	S	4	MAN	C4-C5-C6-O6
3	W	4	MAN	C4-C5-C6-O6
4	Y	4	MAN	C4-C5-C6-O6
3	V	4	MAN	C4-C5-C6-O6
4	Y	4	MAN	O5-C5-C6-O6
3	U	5	MAN	C4-C5-C6-O6
3	U	5	MAN	O5-C5-C6-O6
3	U	4	MAN	C4-C5-C6-O6
3	V	4	MAN	O5-C5-C6-O6
3	R	4	MAN	C4-C5-C6-O6
3	T	4	MAN	C4-C5-C6-O6
3	T	4	MAN	O5-C5-C6-O6
3	R	4	MAN	O5-C5-C6-O6
3	U	4	MAN	O5-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	U	1	NAG	C1-C2-N2-C7
3	X	1	NAG	C1-C2-N2-C7
3	S	5	MAN	C4-C5-C6-O6

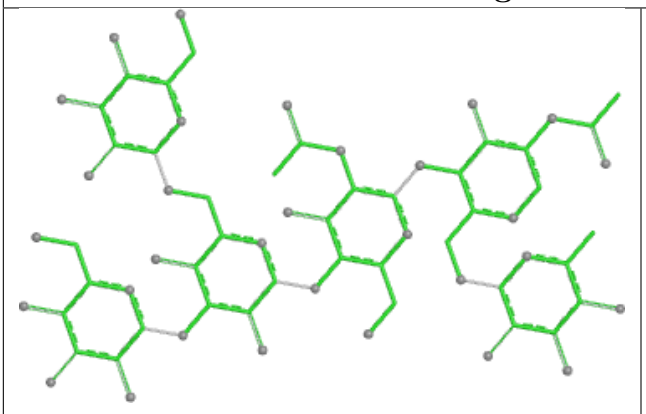
There are no ring outliers.

4 monomers are involved in 5 short contacts:

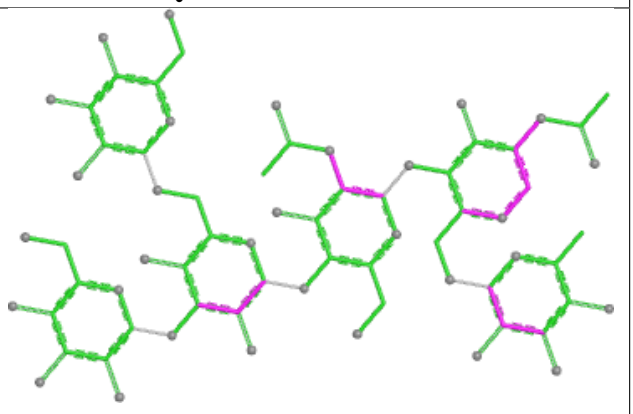
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	W	4	MAN	1	0
3	X	4	MAN	2	0
3	T	4	MAN	1	0
3	Q	6	FUC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

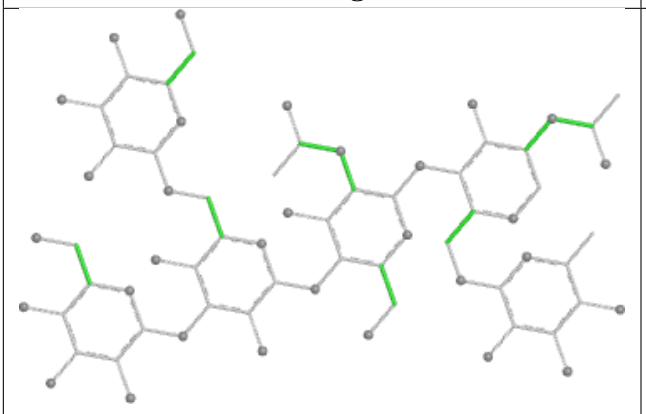
Oligosaccharide Chain Q



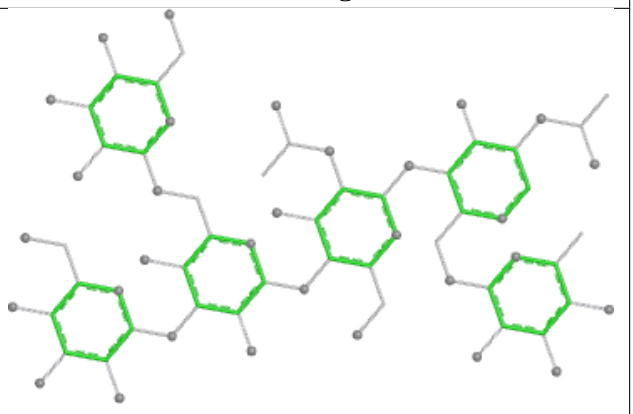
Bond lengths



Bond angles

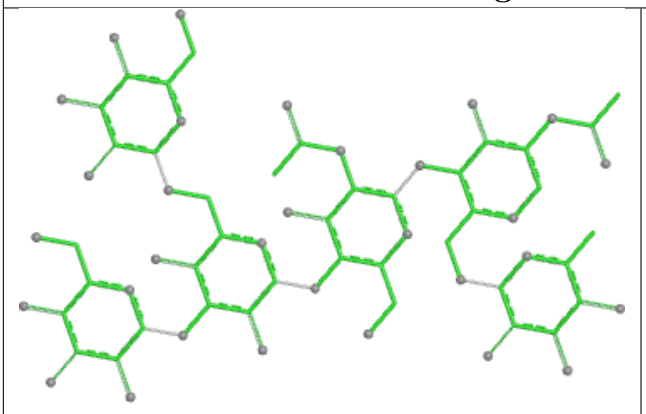


Torsions

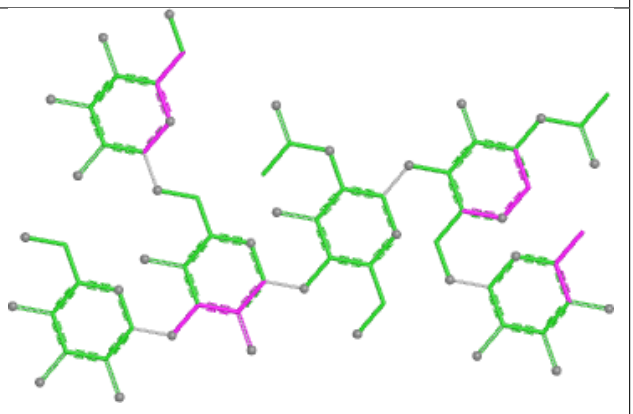


Rings

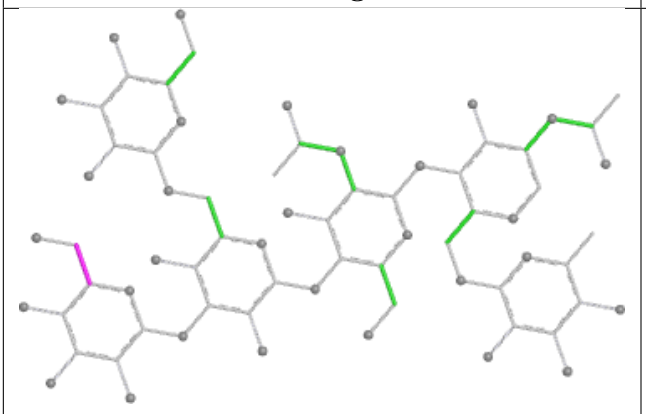
Oligosaccharide Chain R



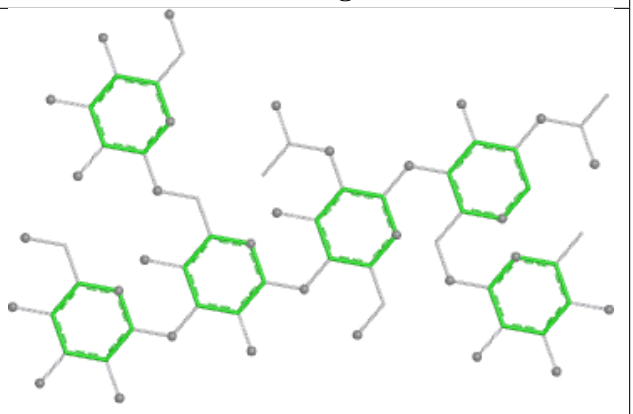
Bond lengths



Bond angles

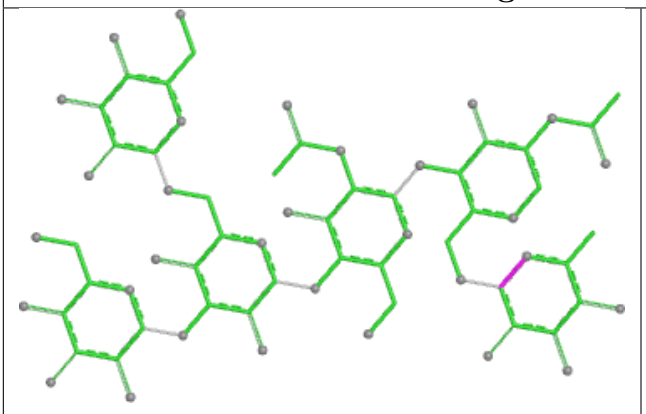


Torsions

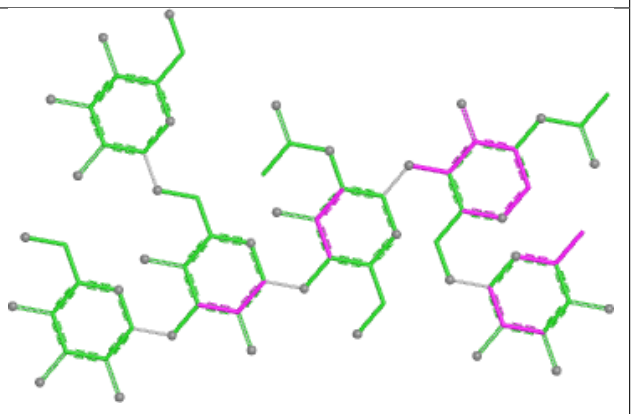


Rings

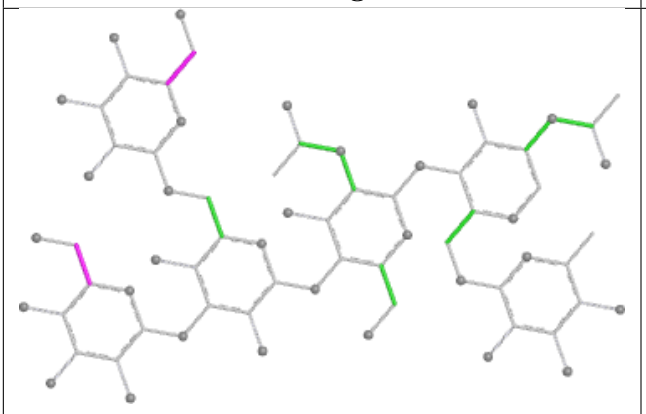
Oligosaccharide Chain S



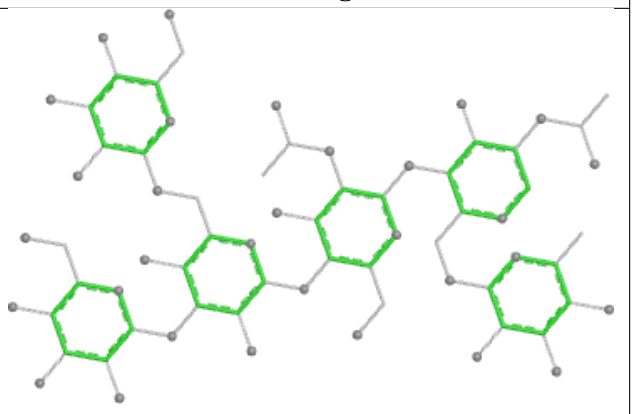
Bond lengths



Bond angles

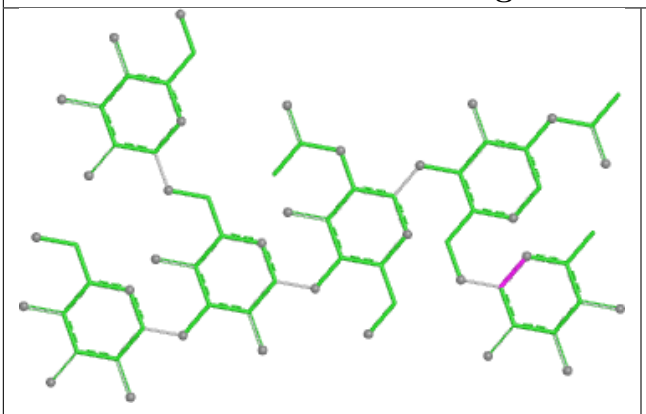


Torsions

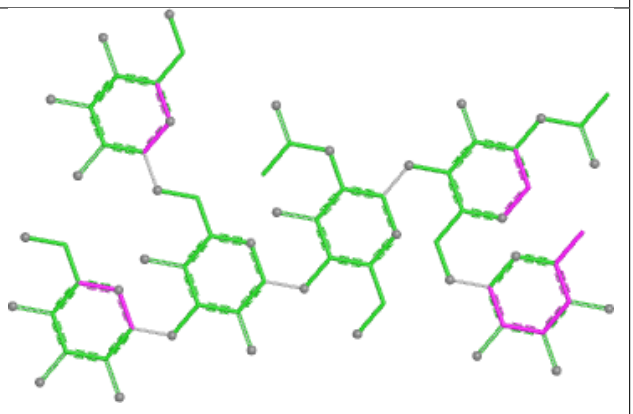


Rings

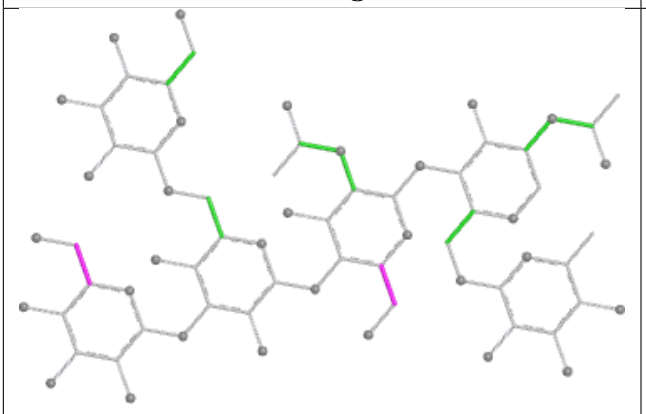
Oligosaccharide Chain T



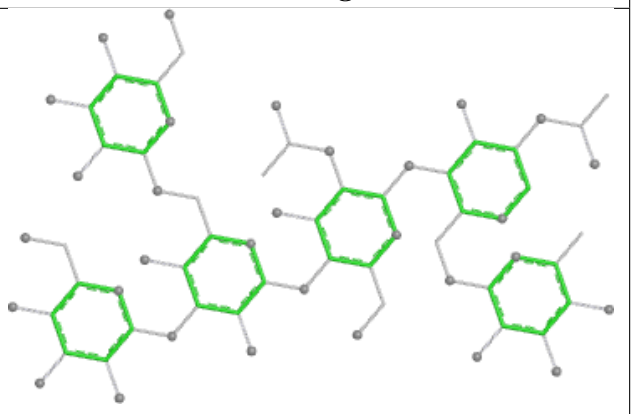
Bond lengths



Bond angles

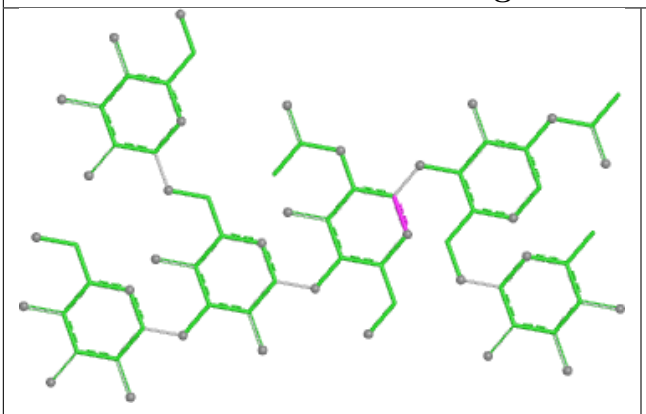


Torsions

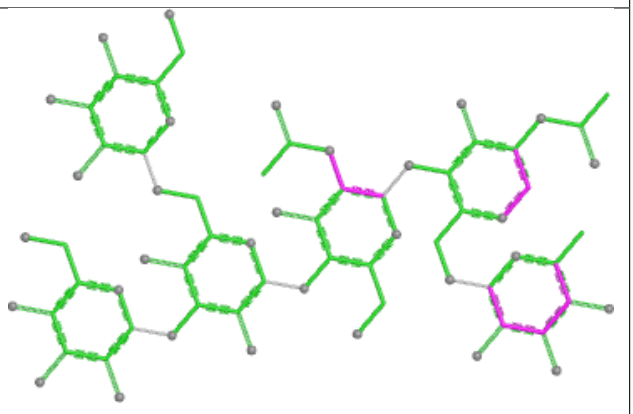


Rings

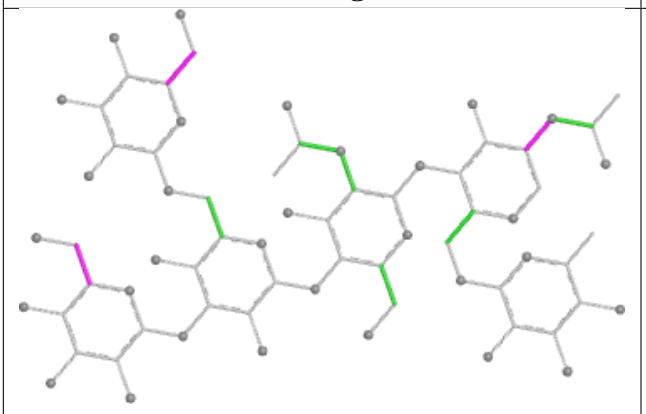
Oligosaccharide Chain U



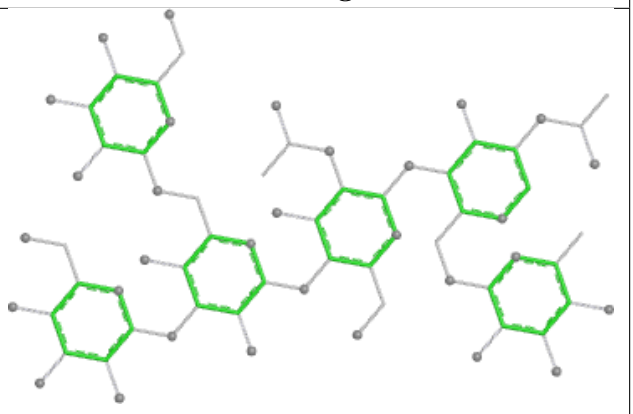
Bond lengths



Bond angles

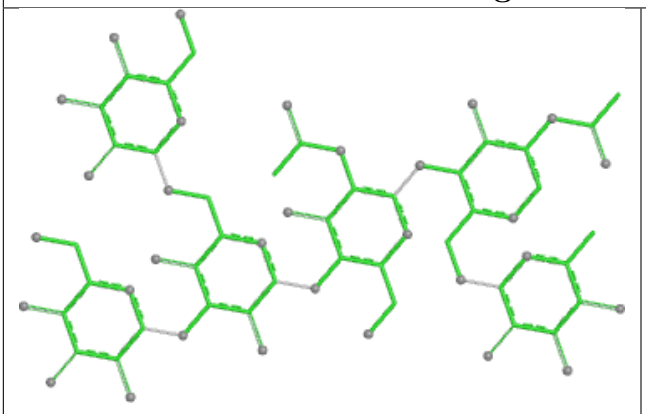


Torsions

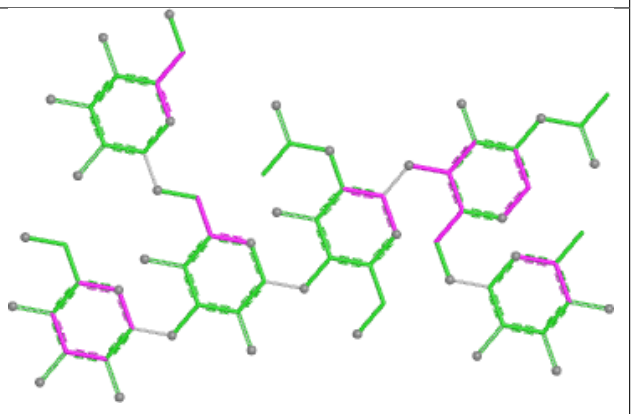


Rings

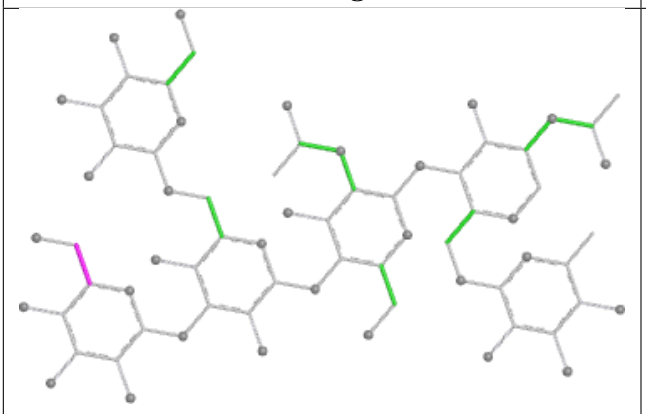
Oligosaccharide Chain V



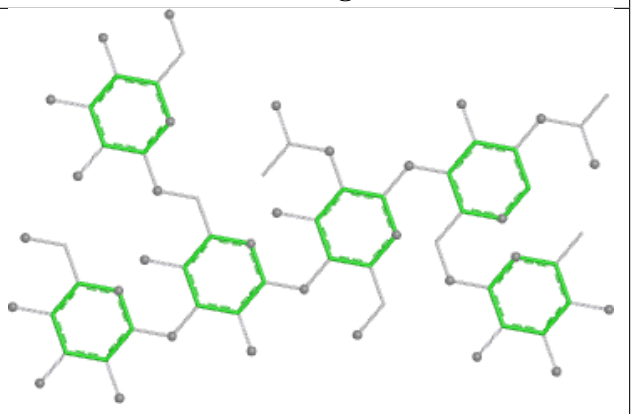
Bond lengths



Bond angles

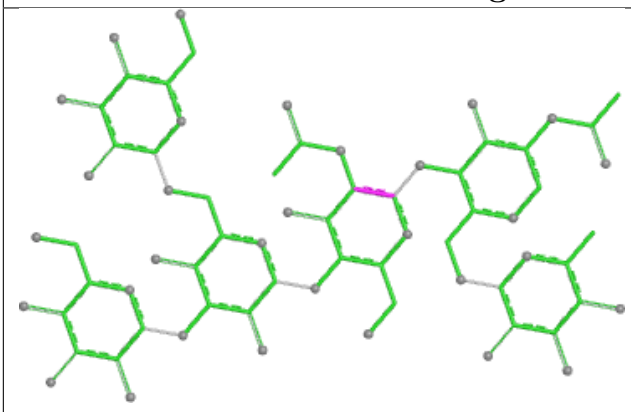


Torsions

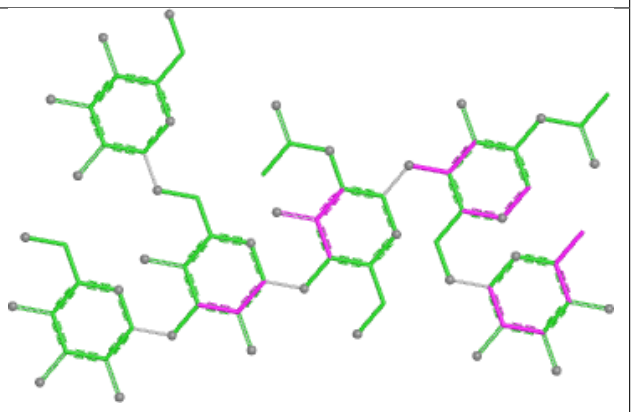


Rings

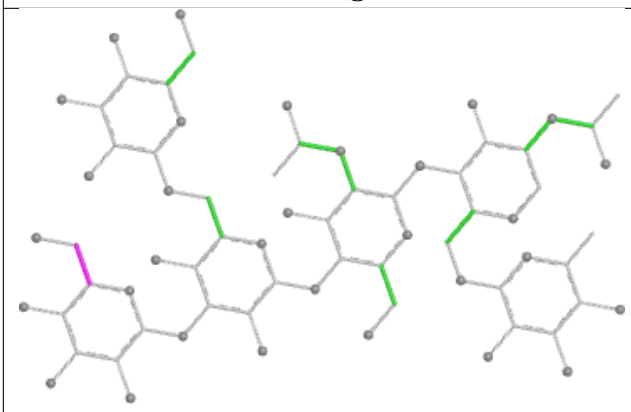
Oligosaccharide Chain W



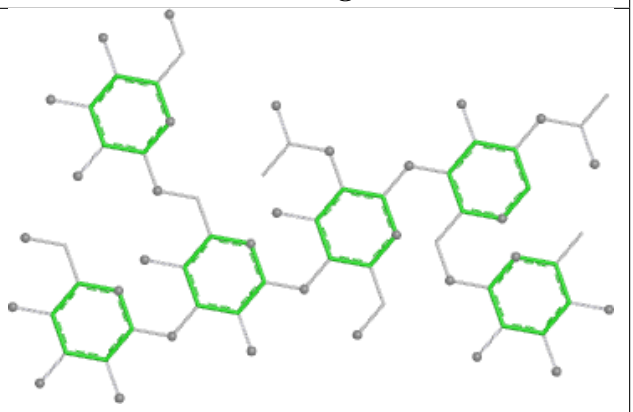
Bond lengths



Bond angles

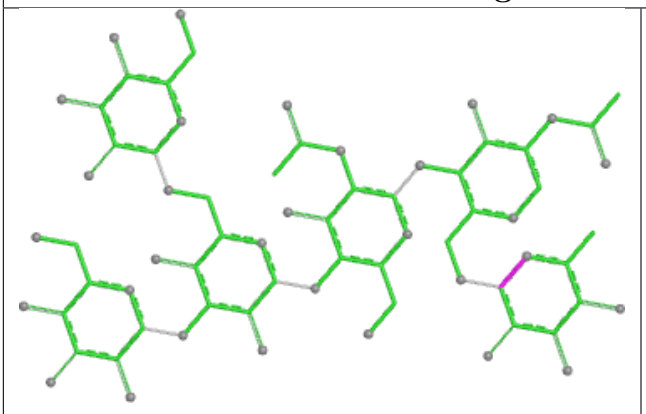


Torsions

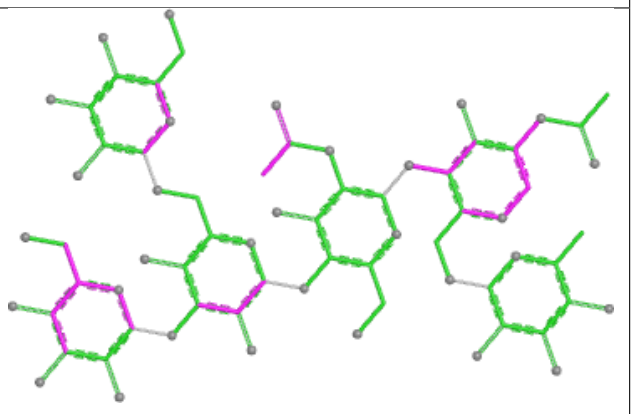


Rings

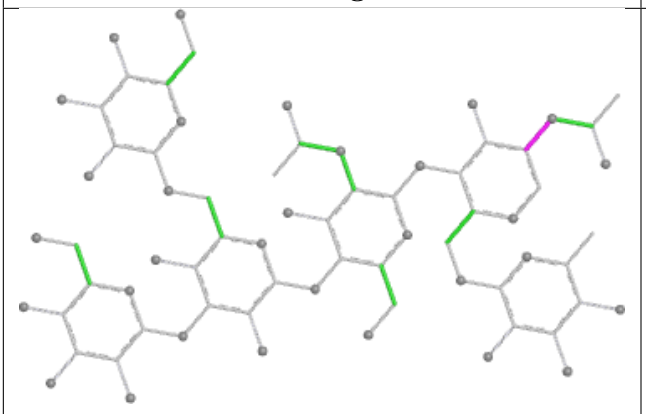
Oligosaccharide Chain X



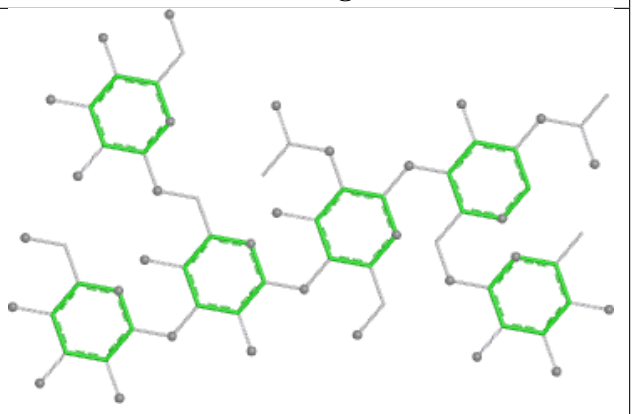
Bond lengths



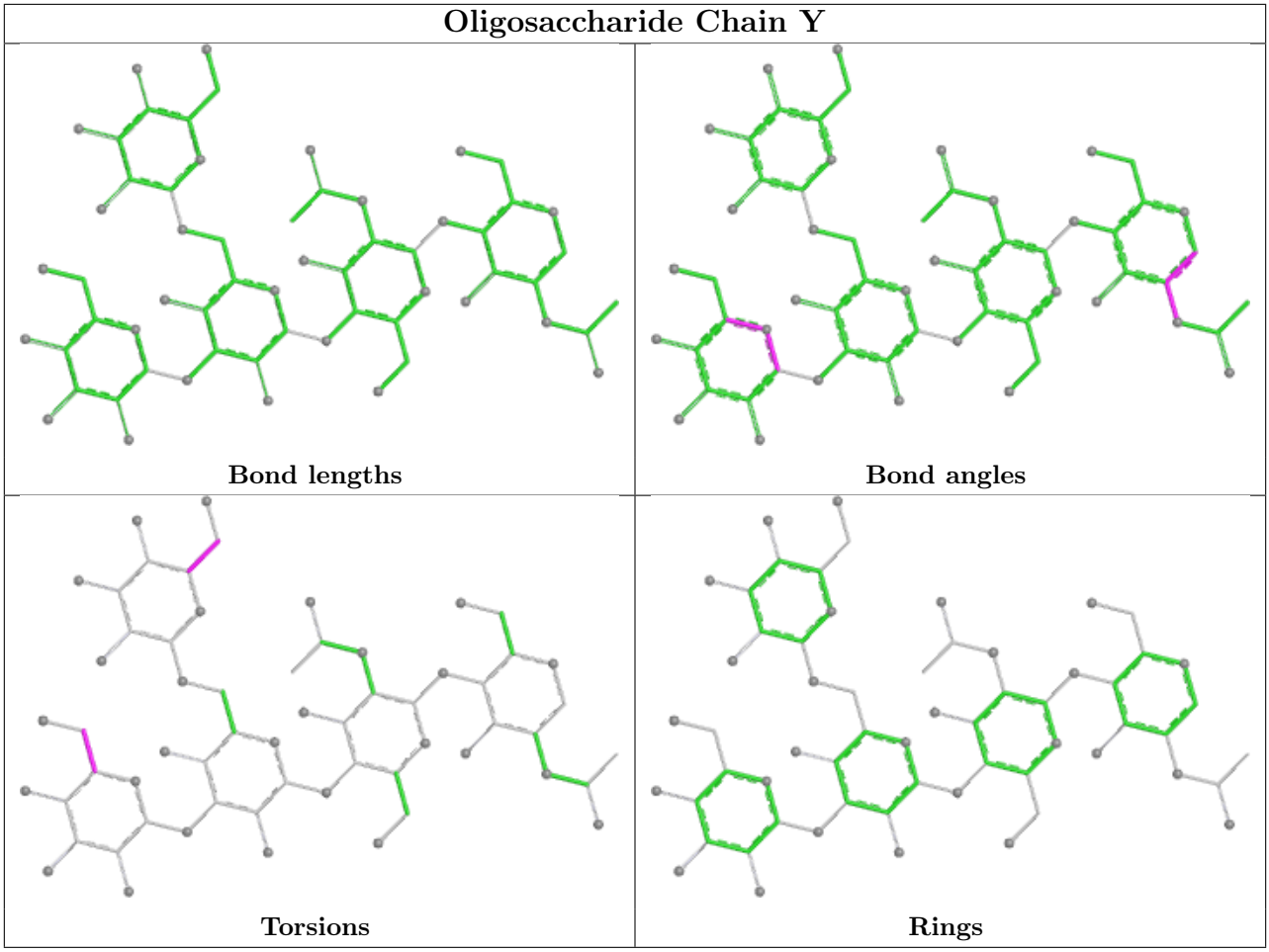
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 47 ligands modelled in this entry, 16 are monoatomic - leaving 31 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	$\#\|Z\| > 2$
7	HEM	P	601	6,2	42,50,50	1.95	7 (16%)	46,82,82	1.60	10 (21%)
6	0KY	G	605	7	14,18,18	2.24	4 (28%)	13,25,25	2.43	5 (38%)
8	NAG	D	604	2	14,14,15	0.58	0	17,19,21	0.94	0
7	HEM	C	602	6,2	42,50,50	1.88	6 (14%)	46,82,82	1.57	6 (13%)
8	NAG	P	603	2	14,14,15	0.49	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	O	603	2	14,14,15	0.49	0	17,19,21	0.81	0
8	NAG	H	603	2	14,14,15	0.46	0	17,19,21	0.64	0
6	0KY	D	602	7	14,18,18	2.31	4 (28%)	13,25,25	2.20	5 (38%)
7	HEM	D	601	6,2,10	42,50,50	1.86	7 (16%)	46,82,82	1.60	7 (15%)
7	HEM	K	601	6,2,10	42,50,50	1.88	6 (14%)	46,82,82	1.66	11 (23%)
7	HEM	L	601	6,2	42,50,50	1.93	8 (19%)	46,82,82	1.89	15 (32%)
8	NAG	C	604	2	14,14,15	0.61	0	17,19,21	1.17	2 (11%)
8	NAG	K	604	2	14,14,15	0.50	0	17,19,21	0.97	1 (5%)
8	NAG	L	604	2	14,14,15	0.70	0	17,19,21	1.05	1 (5%)
7	HEM	H	601	6,2	42,50,50	1.91	6 (14%)	46,82,82	1.61	9 (19%)
8	NAG	H	602	2	14,14,15	0.53	0	17,19,21	1.00	1 (5%)
6	0KY	C	601	7	14,18,18	2.38	4 (28%)	13,25,25	2.48	4 (30%)
6	0KY	O	605	7	14,18,18	2.34	4 (28%)	13,25,25	2.38	4 (30%)
7	HEM	G	601	6,2	42,50,50	1.79	8 (19%)	46,82,82	1.47	7 (15%)
8	NAG	G	602	2	14,14,15	0.61	0	17,19,21	0.84	0
7	HEM	O	601	6,2	42,50,50	1.86	6 (14%)	46,82,82	1.58	9 (19%)
8	NAG	O	602	2	14,14,15	0.53	0	17,19,21	0.79	0
8	NAG	C	603	2	14,14,15	0.55	0	17,19,21	1.14	1 (5%)
8	NAG	D	603	2	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
6	0KY	P	604	7	14,18,18	2.34	4 (28%)	13,25,25	2.33	4 (30%)
8	NAG	K	603	2	14,14,15	0.62	0	17,19,21	1.17	1 (5%)
8	NAG	G	603	2	14,14,15	0.62	0	17,19,21	0.71	0
8	NAG	L	603	2	14,14,15	0.45	0	17,19,21	1.46	2 (11%)
6	0KY	K	602	7	14,18,18	2.26	4 (28%)	13,25,25	2.54	4 (30%)
6	0KY	L	602	7	14,18,18	2.37	4 (28%)	13,25,25	2.29	5 (38%)
6	0KY	H	605	7	14,18,18	2.20	4 (28%)	13,25,25	2.56	6 (46%)

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
7	HEM	P	601	6,2	-	4/12/54/54	-
6	0KY	G	605	7	-	0/7/7/7	0/2/2/2
8	NAG	D	604	2	-	1/6/23/26	0/1/1/1
7	HEM	C	602	6,2	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	P	603	2	-	2/6/23/26	0/1/1/1
8	NAG	O	603	2	-	2/6/23/26	0/1/1/1
8	NAG	H	603	2	-	0/6/23/26	0/1/1/1
6	0KY	D	602	7	-	2/7/7/7	0/2/2/2
7	HEM	D	601	6,2,10	-	6/12/54/54	-
7	HEM	K	601	6,2,10	-	6/12/54/54	-
7	HEM	L	601	6,2	-	6/12/54/54	-
8	NAG	C	604	2	-	2/6/23/26	0/1/1/1
8	NAG	K	604	2	-	2/6/23/26	0/1/1/1
8	NAG	L	604	2	-	2/6/23/26	0/1/1/1
7	HEM	H	601	6,2	-	4/12/54/54	-
8	NAG	H	602	2	-	0/6/23/26	0/1/1/1
6	0KY	C	601	7	-	3/7/7/7	0/2/2/2
6	0KY	O	605	7	-	2/7/7/7	0/2/2/2
7	HEM	G	601	6,2	-	5/12/54/54	-
8	NAG	G	602	2	-	0/6/23/26	0/1/1/1
7	HEM	O	601	6,2	-	6/12/54/54	-
8	NAG	O	602	2	-	0/6/23/26	0/1/1/1
8	NAG	C	603	2	-	0/6/23/26	0/1/1/1
8	NAG	D	603	2	-	1/6/23/26	0/1/1/1
6	0KY	P	604	7	-	3/7/7/7	0/2/2/2
8	NAG	K	603	2	-	0/6/23/26	0/1/1/1
8	NAG	G	603	2	-	2/6/23/26	0/1/1/1
8	NAG	L	603	2	-	2/6/23/26	0/1/1/1
6	0KY	K	602	7	-	3/7/7/7	0/2/2/2
6	0KY	L	602	7	-	2/7/7/7	0/2/2/2
6	0KY	H	605	7	-	4/7/7/7	0/2/2/2

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	601	HEM	C3D-C2D	7.74	1.53	1.36
7	H	601	HEM	C3D-C2D	7.53	1.53	1.36
7	L	601	HEM	C3D-C2D	7.49	1.52	1.36
7	C	602	HEM	C3D-C2D	7.48	1.52	1.36
7	O	601	HEM	C3D-C2D	7.06	1.52	1.36
7	K	601	HEM	C3D-C2D	6.98	1.51	1.36
7	D	601	HEM	C3D-C2D	6.84	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	601	HEM	C3D-C2D	6.50	1.50	1.36
6	O	605	0KY	O2-C8	5.78	1.36	1.23
6	P	604	0KY	O2-C8	5.76	1.36	1.23
6	C	601	0KY	O2-C8	5.74	1.36	1.23
6	H	605	0KY	O2-C8	5.71	1.36	1.23
6	L	602	0KY	O2-C8	5.64	1.36	1.23
6	K	602	0KY	O2-C8	5.58	1.36	1.23
6	D	602	0KY	O2-C8	5.57	1.36	1.23
6	G	605	0KY	O2-C8	5.48	1.36	1.23
7	G	601	HEM	C3C-C2C	-4.87	1.33	1.40
7	P	601	HEM	C3C-C2C	-4.50	1.34	1.40
7	D	601	HEM	C3C-C2C	-4.44	1.34	1.40
6	C	601	0KY	C9-N1	4.39	1.44	1.38
6	L	602	0KY	C9-N1	4.31	1.43	1.38
7	K	601	HEM	C3C-C4C	4.29	1.47	1.41
7	K	601	HEM	C3C-C2C	-4.25	1.34	1.40
7	C	602	HEM	C3C-C2C	-4.24	1.34	1.40
6	D	602	0KY	C9-N1	4.08	1.43	1.38
6	K	602	0KY	C9-N1	4.07	1.43	1.38
7	H	601	HEM	C3C-C2C	-4.06	1.34	1.40
6	O	605	0KY	C9-N1	4.02	1.43	1.38
7	O	601	HEM	C3C-C2C	-3.95	1.35	1.40
6	H	605	0KY	C9-N1	3.90	1.43	1.38
6	P	604	0KY	C9-N1	3.82	1.43	1.38
7	L	601	HEM	C3C-C2C	-3.78	1.35	1.40
6	G	605	0KY	C9-N1	3.61	1.42	1.38
6	G	605	0KY	C6-N1	-3.55	1.33	1.39
7	D	601	HEM	C3C-CAC	3.54	1.55	1.47
7	P	601	HEM	C3C-CAC	3.54	1.55	1.47
7	L	601	HEM	C3C-C4C	3.54	1.46	1.41
7	H	601	HEM	C3C-C4C	3.46	1.46	1.41
6	P	604	0KY	C6-N1	-3.45	1.34	1.39
6	C	601	0KY	C6-N1	-3.39	1.34	1.39
7	L	601	HEM	C3C-CAC	3.35	1.55	1.47
7	L	601	HEM	FE-ND	3.34	2.16	1.98
6	D	602	0KY	C6-N1	-3.30	1.34	1.39
6	O	605	0KY	C9-S	3.29	1.73	1.67
6	L	602	0KY	C9-S	3.24	1.73	1.67
6	P	604	0KY	C9-S	3.23	1.73	1.67
7	G	601	HEM	CAB-C3B	3.23	1.56	1.47
7	D	601	HEM	CAB-C3B	3.21	1.56	1.47
6	L	602	0KY	C6-N1	-3.21	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	601	HEM	CAB-C3B	3.21	1.55	1.47
6	K	602	0KY	C6-N1	-3.17	1.34	1.39
6	D	602	0KY	C9-S	3.15	1.73	1.67
7	C	602	HEM	CAB-C3B	3.12	1.55	1.47
7	O	601	HEM	C3C-C4C	3.10	1.45	1.41
7	P	601	HEM	CAB-C3B	3.08	1.55	1.47
6	O	605	0KY	C6-N1	-3.08	1.34	1.39
7	O	601	HEM	C3C-CAC	3.06	1.54	1.47
7	H	601	HEM	CAB-C3B	3.03	1.55	1.47
6	G	605	0KY	C9-S	2.99	1.72	1.67
6	H	605	0KY	C9-S	2.96	1.72	1.67
7	L	601	HEM	CAB-C3B	2.95	1.55	1.47
7	K	601	HEM	CAB-C3B	2.94	1.55	1.47
7	K	601	HEM	C3C-CAC	2.89	1.54	1.47
7	C	602	HEM	C3C-CAC	2.87	1.54	1.47
7	C	602	HEM	C3C-C4C	2.81	1.45	1.41
7	H	601	HEM	C3C-CAC	2.75	1.53	1.47
6	C	601	0KY	C9-S	2.74	1.72	1.67
7	G	601	HEM	C3C-CAC	2.64	1.53	1.47
6	K	602	0KY	C9-S	2.56	1.72	1.67
7	D	601	HEM	C3C-C4C	2.46	1.45	1.41
7	K	601	HEM	FE-ND	2.43	2.11	1.98
6	H	605	0KY	C6-N1	-2.42	1.35	1.39
7	P	601	HEM	C3C-C4C	2.36	1.44	1.41
7	G	601	HEM	CMB-C2B	2.32	1.55	1.50
7	C	602	HEM	FE-ND	2.21	2.10	1.98
7	H	601	HEM	FE-ND	2.18	2.10	1.98
7	L	601	HEM	CMB-C2B	2.17	1.55	1.50
7	G	601	HEM	O2A-CGA	-2.10	1.23	1.30
7	O	601	HEM	CMA-C3A	2.08	1.55	1.51
7	L	601	HEM	CMD-C2D	2.08	1.55	1.50
7	P	601	HEM	FE-ND	2.05	2.09	1.98
7	D	601	HEM	CMD-C2D	2.04	1.55	1.50
7	G	601	HEM	C3B-C2B	-2.04	1.33	1.37
7	D	601	HEM	CMC-C2C	2.04	1.56	1.51
7	P	601	HEM	CMD-C2D	2.02	1.54	1.50
7	G	601	HEM	C3C-C4C	2.01	1.44	1.41

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	602	0KY	C6-N1-C9	-7.06	117.00	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	601	0KY	C6-N1-C9	-6.63	117.28	121.53
6	O	605	0KY	C6-N1-C9	-6.10	117.62	121.53
6	P	604	0KY	C6-N1-C9	-6.04	117.66	121.53
6	H	605	0KY	C6-N1-C9	-5.81	117.81	121.53
6	L	602	0KY	C6-N1-C9	-5.59	117.95	121.53
6	G	605	0KY	C6-N1-C9	-5.44	118.04	121.53
6	D	602	0KY	C6-N1-C9	-5.31	118.13	121.53
7	P	601	HEM	C4D-ND-C1D	4.97	111.09	105.21
7	L	601	HEM	C4D-ND-C1D	4.96	111.09	105.21
7	H	601	HEM	C4D-ND-C1D	4.59	110.65	105.21
6	G	605	0KY	S-C9-N1	-4.40	119.54	123.43
7	K	601	HEM	C4D-ND-C1D	4.26	110.25	105.21
7	D	601	HEM	C4D-ND-C1D	4.08	110.03	105.21
7	C	602	HEM	C4D-ND-C1D	4.07	110.02	105.21
6	H	605	0KY	S-C9-N1	-4.05	119.85	123.43
7	O	601	HEM	C4D-ND-C1D	3.94	109.88	105.21
8	L	603	NAG	C1-O5-C5	3.79	117.26	112.19
7	L	601	HEM	C4C-CHD-C1D	3.77	127.53	122.56
6	L	602	0KY	C10-N3-C7	3.76	108.96	102.55
7	H	601	HEM	C4C-CHD-C1D	3.71	127.45	122.56
7	D	601	HEM	C4C-CHD-C1D	3.61	127.33	122.56
6	C	601	0KY	C10-N3-C7	3.59	108.66	102.55
6	O	605	0KY	C10-N3-C7	3.58	108.64	102.55
6	D	602	0KY	C10-N3-C7	3.57	108.62	102.55
7	G	601	HEM	C4D-ND-C1D	3.51	109.37	105.21
6	H	605	0KY	C10-N3-C7	3.44	108.40	102.55
6	P	604	0KY	C10-N3-C7	3.43	108.38	102.55
6	K	602	0KY	C10-N3-C7	3.42	108.37	102.55
7	L	601	HEM	C3B-C4B-NB	-3.41	107.02	109.47
7	D	601	HEM	C3B-C2B-C1B	3.41	108.97	106.41
6	G	605	0KY	C10-N3-C7	3.31	108.18	102.55
7	G	601	HEM	CMA-C3A-C4A	-3.28	123.65	128.46
7	P	601	HEM	C4B-CHC-C1C	3.27	126.88	122.56
7	K	601	HEM	C4C-CHD-C1D	3.25	126.85	122.56
7	L	601	HEM	CMD-C2D-C1D	3.19	130.02	125.03
7	L	601	HEM	CBA-CAA-C2A	-3.18	107.19	112.54
7	G	601	HEM	C4C-CHD-C1D	3.18	126.75	122.56
7	C	602	HEM	CMA-C3A-C4A	-3.16	123.82	128.46
7	O	601	HEM	CMD-C2D-C1D	3.16	129.97	125.03
6	H	605	0KY	C10-N4-C6	3.15	107.53	101.92
7	G	601	HEM	CBA-CAA-C2A	-3.08	107.36	112.54
6	O	605	0KY	S-C9-N1	-3.07	120.71	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	601	HEM	CMD-C2D-C1D	2.98	129.69	125.03
6	P	604	0KY	S-C9-N1	-2.98	120.80	123.43
6	L	602	0KY	C10-N4-C6	2.95	107.19	101.92
7	C	602	HEM	C3B-C2B-C1B	2.90	108.59	106.41
6	O	605	0KY	C10-N4-C6	2.89	107.08	101.92
7	K	601	HEM	C3B-C2B-C1B	2.89	108.58	106.41
7	K	601	HEM	CMC-C2C-C3C	2.85	130.39	124.68
6	D	602	0KY	C10-N4-C6	2.85	107.00	101.92
6	K	602	0KY	C10-N4-C6	2.84	106.98	101.92
7	H	601	HEM	CMA-C3A-C4A	-2.84	124.30	128.46
7	C	602	HEM	C4B-CHC-C1C	2.82	126.29	122.56
7	D	601	HEM	CMD-C2D-C1D	2.82	129.45	125.03
7	L	601	HEM	C3B-C2B-C1B	2.80	108.51	106.41
7	L	601	HEM	C4B-CHC-C1C	2.79	126.24	122.56
6	C	601	0KY	C10-N4-C6	2.78	106.88	101.92
7	O	601	HEM	CHC-C4B-NB	2.75	127.39	124.44
7	O	601	HEM	C4C-CHD-C1D	2.72	126.15	122.56
7	L	601	HEM	C1B-NB-C4B	2.71	108.41	105.21
7	H	601	HEM	C3B-C2B-C1B	2.70	108.44	106.41
7	P	601	HEM	CBA-CAA-C2A	-2.69	108.02	112.54
6	P	604	0KY	C10-N4-C6	2.65	106.65	101.92
7	H	601	HEM	CMC-C2C-C3C	2.61	129.90	124.68
7	L	601	HEM	CHB-C1B-NB	2.61	127.60	124.37
7	K	601	HEM	CHB-C1B-NB	2.60	127.60	124.37
6	L	602	0KY	S-C9-N1	-2.58	121.14	123.43
7	G	601	HEM	CHD-C1D-ND	2.55	127.18	124.44
7	O	601	HEM	CAD-C3D-C4D	2.53	129.12	124.70
7	K	601	HEM	CAD-C3D-C4D	2.51	129.08	124.70
7	L	601	HEM	CMA-C3A-C4A	-2.51	124.78	128.46
7	H	601	HEM	CMD-C2D-C1D	2.49	128.93	125.03
7	C	602	HEM	CAD-C3D-C4D	2.49	129.04	124.70
7	K	601	HEM	C3C-C4C-NC	-2.45	106.31	110.94
7	O	601	HEM	CHB-C1B-NB	2.45	127.41	124.37
8	C	603	NAG	C1-O5-C5	2.45	115.47	112.19
7	P	601	HEM	C1B-NB-C4B	2.44	108.10	105.21
6	K	602	0KY	S-C9-N1	-2.44	121.27	123.43
6	G	605	0KY	C10-N4-C6	2.42	106.24	101.92
7	D	601	HEM	CMA-C3A-C4A	-2.41	124.92	128.46
7	C	602	HEM	C4A-C3A-C2A	2.41	108.67	107.00
7	H	601	HEM	C4A-C3A-C2A	2.40	108.67	107.00
7	P	601	HEM	C3B-C2B-C1B	2.39	108.21	106.41
7	G	601	HEM	CAD-C3D-C4D	2.38	128.85	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	604	NAG	O7-C7-C8	-2.36	117.85	122.05
7	O	601	HEM	C3B-C2B-C1B	2.35	108.17	106.41
7	P	601	HEM	C4A-C3A-C2A	2.32	108.61	107.00
7	K	601	HEM	CMA-C3A-C4A	-2.30	125.09	128.46
7	K	601	HEM	C4B-CHC-C1C	2.30	125.59	122.56
7	L	601	HEM	C3C-C4C-NC	-2.28	106.63	110.94
7	L	601	HEM	C2C-C3C-C4C	2.26	108.48	106.90
8	D	603	NAG	O4-C4-C5	2.22	114.80	109.32
7	P	601	HEM	C3B-C4B-NB	-2.22	107.88	109.47
6	D	602	0KY	S-C9-N1	-2.20	121.48	123.43
7	O	601	HEM	C3B-C4B-NB	-2.19	107.89	109.47
7	H	601	HEM	C3C-C4C-NC	-2.18	106.83	110.94
7	O	601	HEM	C2C-C3C-C4C	2.17	108.41	106.90
7	G	601	HEM	C3B-C2B-C1B	2.15	108.02	106.41
8	L	604	NAG	O5-C5-C4	-2.14	105.61	110.83
8	P	603	NAG	C3-C4-C5	-2.14	106.35	110.23
8	K	603	NAG	O7-C7-C8	-2.14	118.25	122.05
6	G	605	0KY	O2-C8-C7	-2.13	120.10	124.32
8	K	604	NAG	O7-C7-C8	-2.12	118.28	122.05
7	K	601	HEM	CBA-CAA-C2A	-2.12	108.97	112.54
7	L	601	HEM	CAD-C3D-C4D	2.12	128.39	124.70
7	L	601	HEM	CMC-C2C-C3C	2.12	128.91	124.68
7	D	601	HEM	O2A-CGA-CBA	2.11	120.66	114.00
6	H	605	0KY	C5-N1-C6	2.10	121.74	119.36
6	C	601	0KY	S-C9-N1	-2.10	121.57	123.43
8	L	603	NAG	O5-C1-C2	-2.07	108.08	111.29
7	H	601	HEM	CHC-C4B-NB	2.07	126.66	124.44
8	C	604	NAG	C1-C2-N2	-2.07	107.18	110.43
7	D	601	HEM	O1A-CGA-CBA	-2.06	116.57	123.09
6	H	605	0KY	C7-C8-N2	2.05	117.98	114.07
7	P	601	HEM	C4C-CHD-C1D	2.04	125.25	122.56
7	P	601	HEM	CMA-C3A-C4A	-2.04	125.47	128.46
6	L	602	0KY	C7-C8-N2	2.04	117.95	114.07
7	P	601	HEM	CAD-C3D-C4D	2.02	128.23	124.70
7	L	601	HEM	C2B-C1B-NB	-2.02	107.52	109.84
8	H	602	NAG	C1-C2-N2	-2.01	107.26	110.43
6	D	602	0KY	C7-C8-N2	2.00	117.89	114.07

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	601	0KY	C3-C5-N1-C9
6	D	602	0KY	O1-C3-C5-N1
6	H	605	0KY	C3-C5-N1-C9
6	H	605	0KY	O1-C3-C5-N1
6	H	605	0KY	C1-C2-O1-C3
6	K	602	0KY	C3-C5-N1-C9
6	K	602	0KY	O1-C3-C5-N1
6	L	602	0KY	O1-C3-C5-N1
6	L	602	0KY	C4-C3-C5-N1
6	O	605	0KY	O1-C3-C5-N1
6	O	605	0KY	C4-C3-C5-N1
8	C	604	NAG	O5-C5-C6-O6
8	O	603	NAG	O5-C5-C6-O6
8	C	604	NAG	C4-C5-C6-O6
6	P	604	0KY	C1-C2-O1-C3
8	O	603	NAG	C4-C5-C6-O6
8	L	604	NAG	C4-C5-C6-O6
8	L	604	NAG	O5-C5-C6-O6
8	P	603	NAG	C4-C5-C6-O6
8	L	603	NAG	C4-C5-C6-O6
8	L	603	NAG	O5-C5-C6-O6
8	P	603	NAG	O5-C5-C6-O6
7	K	601	HEM	C2B-C3B-CAB-CBB
7	L	601	HEM	C2B-C3B-CAB-CBB
6	C	601	0KY	C4-C3-C5-N1
6	D	602	0KY	C4-C3-C5-N1
6	H	605	0KY	C4-C3-C5-N1
6	K	602	0KY	C4-C3-C5-N1
8	K	604	NAG	C4-C5-C6-O6
8	G	603	NAG	C3-C2-N2-C7
7	O	601	HEM	C3A-C2A-CAA-CBA
7	O	601	HEM	C1A-C2A-CAA-CBA
8	K	604	NAG	O5-C5-C6-O6
6	C	601	0KY	O1-C3-C5-N1
6	P	604	0KY	O1-C3-C5-N1
7	D	601	HEM	C3A-C2A-CAA-CBA
6	P	604	0KY	C4-C3-C5-N1
7	G	601	HEM	CAD-CBD-CGD-O1D
7	G	601	HEM	CAD-CBD-CGD-O2D
7	K	601	HEM	CAD-CBD-CGD-O1D
7	K	601	HEM	CAA-CBA-CGA-O2A
7	K	601	HEM	CAA-CBA-CGA-O1A
7	D	601	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
7	G	601	HEM	CAA-CBA-CGA-O1A
7	G	601	HEM	CAA-CBA-CGA-O2A
7	H	601	HEM	CAA-CBA-CGA-O1A
7	O	601	HEM	CAA-CBA-CGA-O1A
7	P	601	HEM	CAD-CBD-CGD-O1D
7	P	601	HEM	CAD-CBD-CGD-O2D
7	C	602	HEM	CAD-CBD-CGD-O1D
7	O	601	HEM	CAA-CBA-CGA-O2A
7	C	602	HEM	CAA-CBA-CGA-O2A
7	C	602	HEM	CAD-CBD-CGD-O2D
7	H	601	HEM	CAA-CBA-CGA-O2A
7	K	601	HEM	CAD-CBD-CGD-O2D
7	O	601	HEM	CAD-CBD-CGD-O1D
7	O	601	HEM	CAD-CBD-CGD-O2D
7	D	601	HEM	CAA-CBA-CGA-O1A
7	C	602	HEM	CAA-CBA-CGA-O1A
7	H	601	HEM	CAD-CBD-CGD-O1D
8	D	604	NAG	C1-C2-N2-C7
8	G	603	NAG	C1-C2-N2-C7
7	L	601	HEM	CAA-CBA-CGA-O1A
7	D	601	HEM	CAD-CBD-CGD-O1D
7	L	601	HEM	CAD-CBD-CGD-O2D
7	L	601	HEM	CAD-CBD-CGD-O1D
7	D	601	HEM	CAD-CBD-CGD-O2D
7	P	601	HEM	CAA-CBA-CGA-O2A
7	G	601	HEM	C4B-C3B-CAB-CBB
7	K	601	HEM	C4B-C3B-CAB-CBB
7	L	601	HEM	C4B-C3B-CAB-CBB
7	P	601	HEM	CAA-CBA-CGA-O1A
7	L	601	HEM	CAA-CBA-CGA-O2A
7	H	601	HEM	CAD-CBD-CGD-O2D
8	D	603	NAG	C4-C5-C6-O6
7	D	601	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

18 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	601	HEM	7	0
6	G	605	0KY	1	0
8	D	604	NAG	1	0
7	C	602	HEM	6	0

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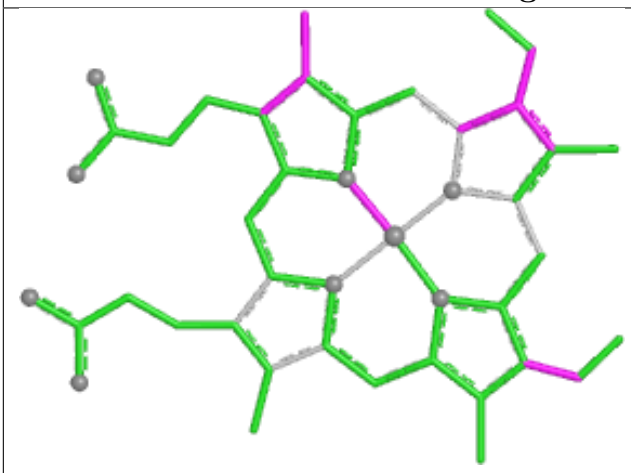
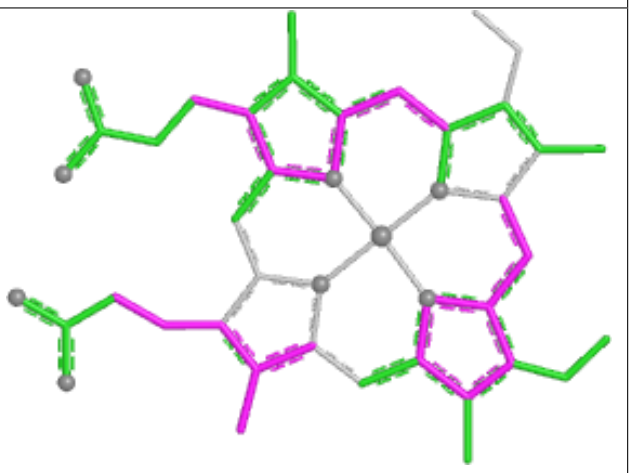
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	602	0KY	4	0
7	D	601	HEM	5	0
7	K	601	HEM	1	0
7	L	601	HEM	5	0
7	H	601	HEM	5	0
6	C	601	0KY	3	0
6	O	605	0KY	5	0
7	G	601	HEM	6	0
7	O	601	HEM	5	0
6	P	604	0KY	4	0
8	G	603	NAG	2	0
6	K	602	0KY	2	0
6	L	602	0KY	1	0
6	H	605	0KY	5	0

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 then 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.

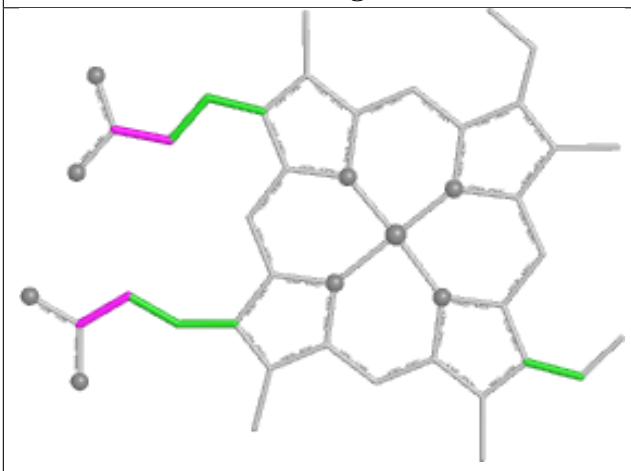
Ligand HEM P 601



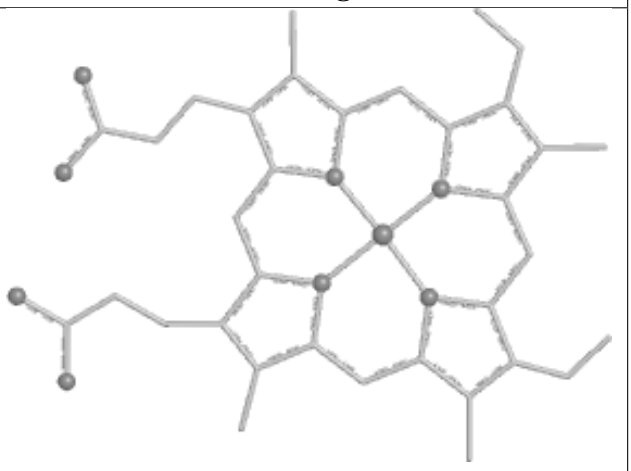
Bond lengths



Bond angles

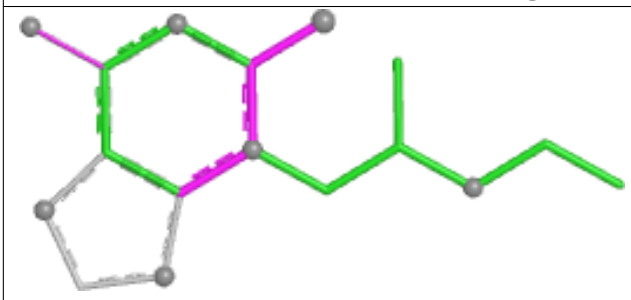


Torsions



Rings

Ligand 0KY G 605



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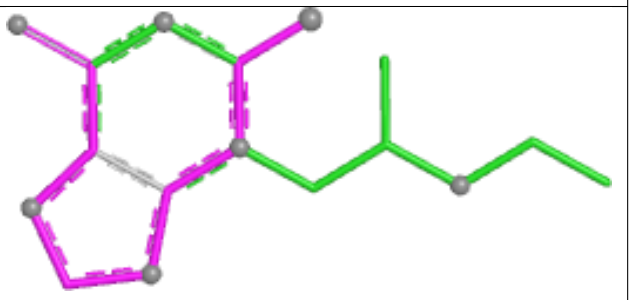

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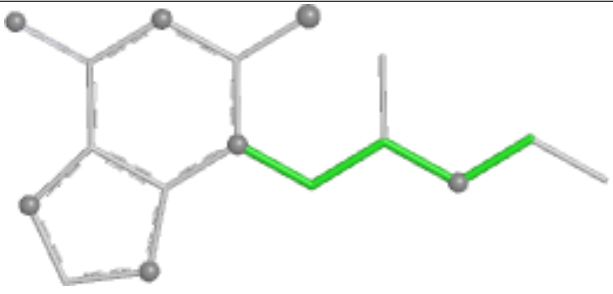

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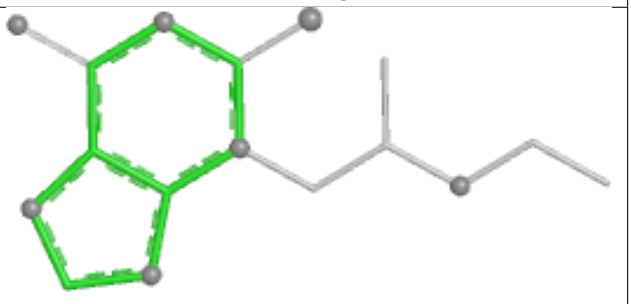
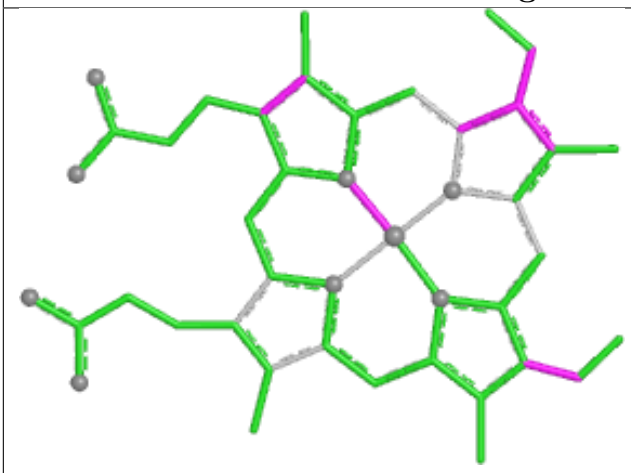


Rings

Ligand HEM C 602



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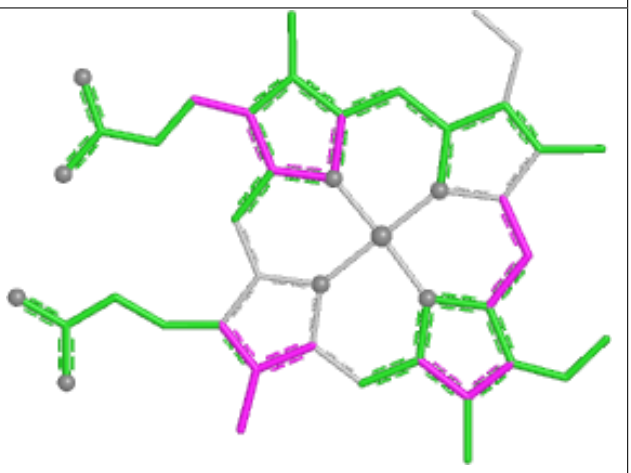
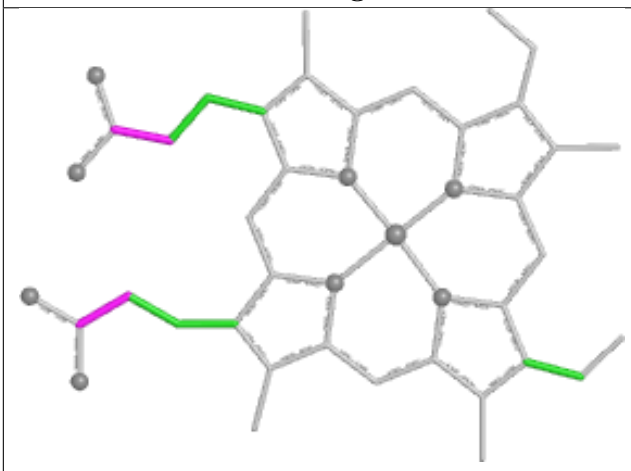


Bond angles



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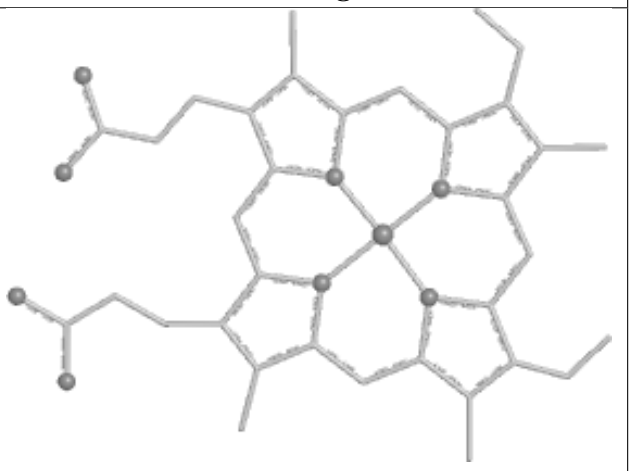
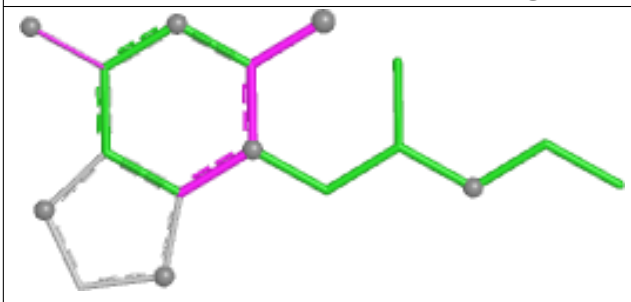


Rings

Ligand 0KY D 602



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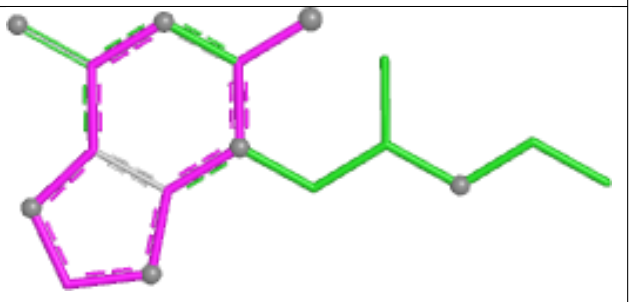
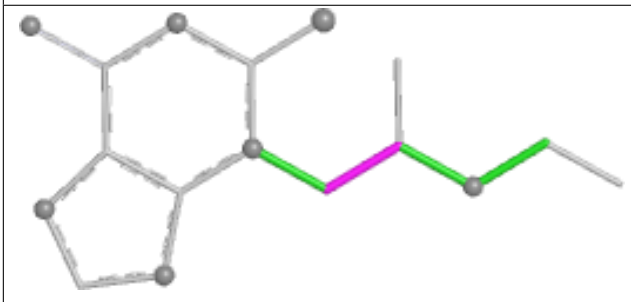


Bond angles



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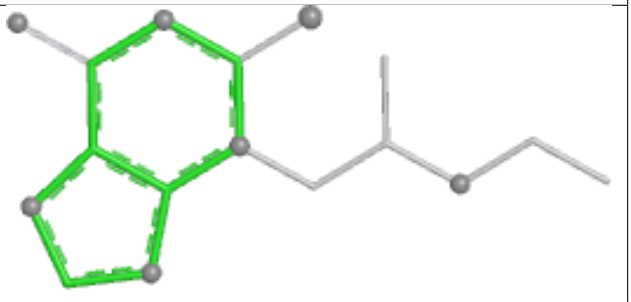
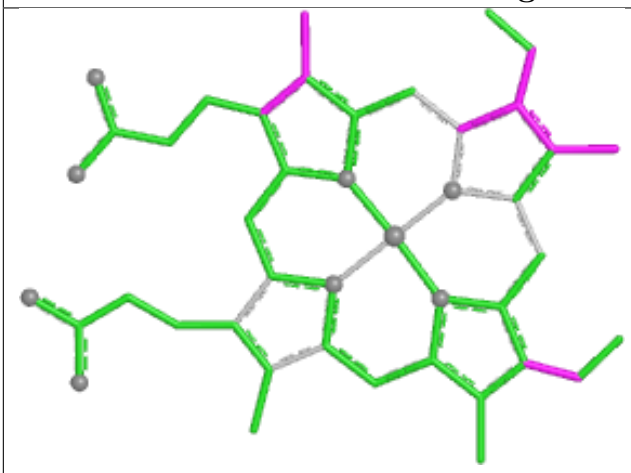


Rings

Ligand HEM D 601



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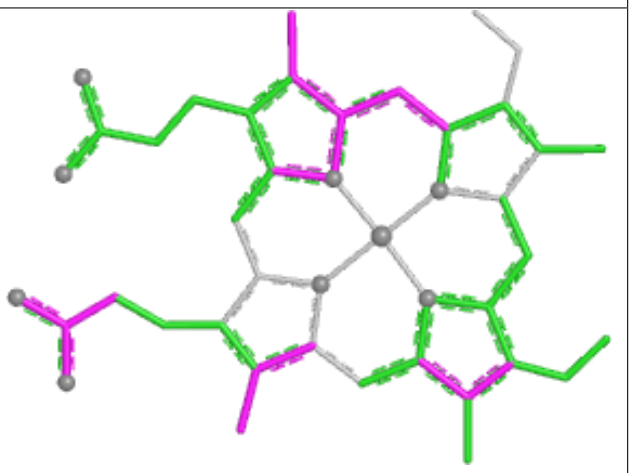

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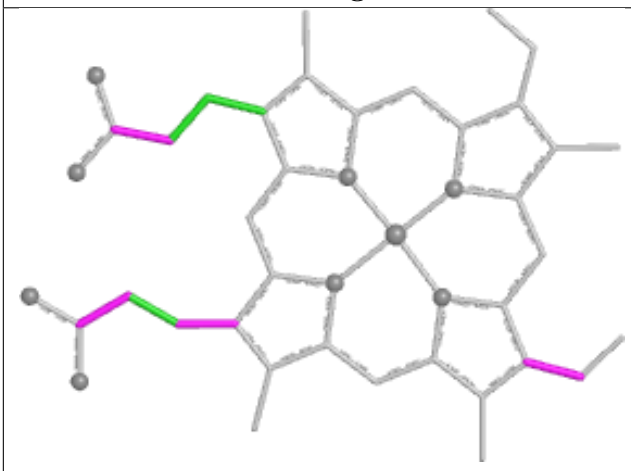

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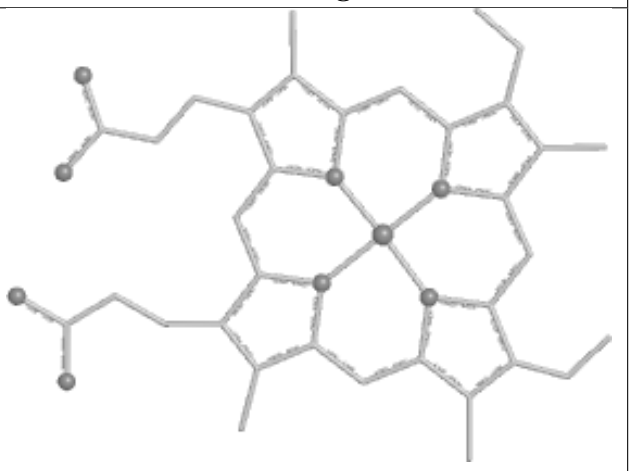
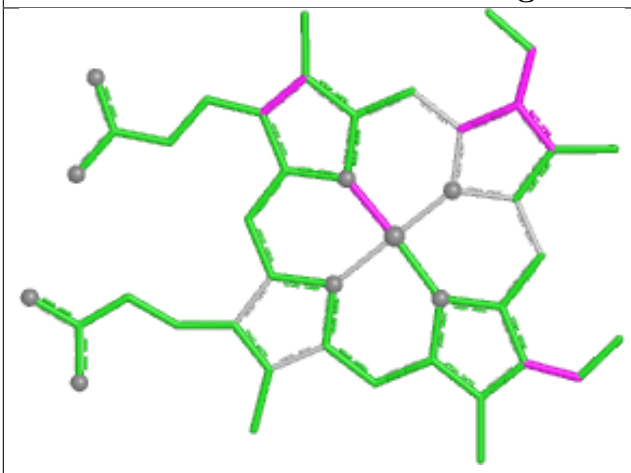


Rings

Ligand HEM K 601



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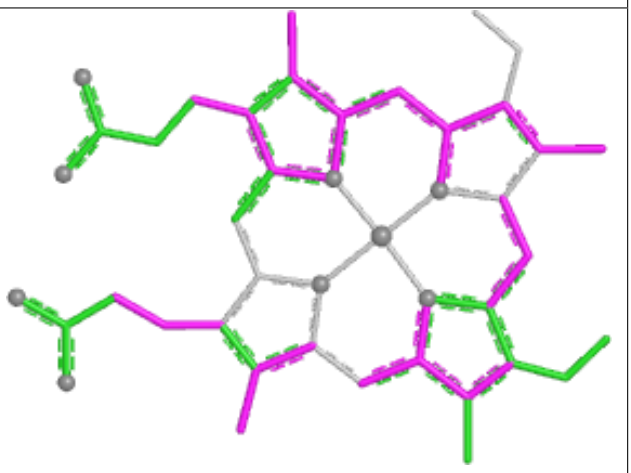

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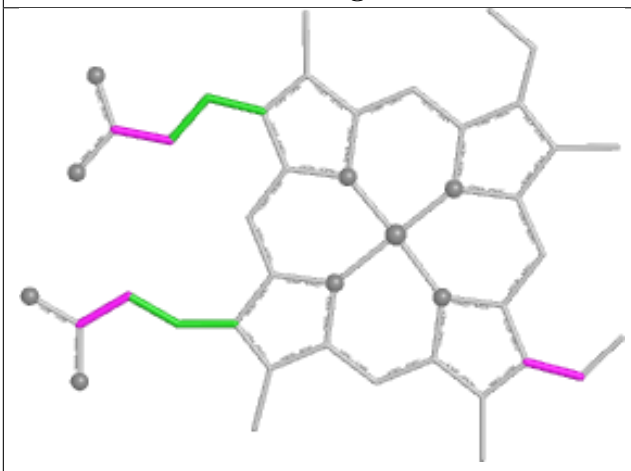

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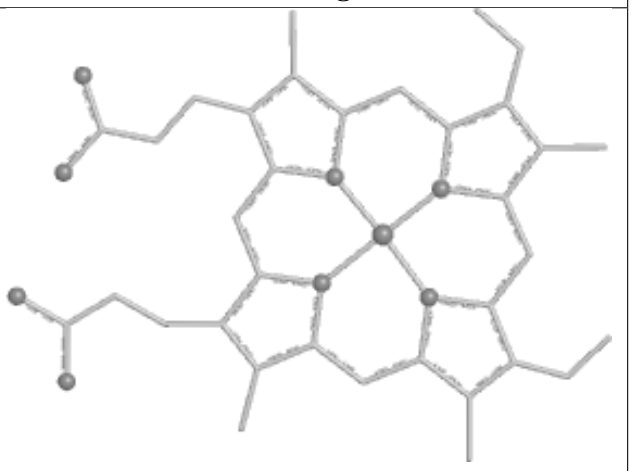

Rings

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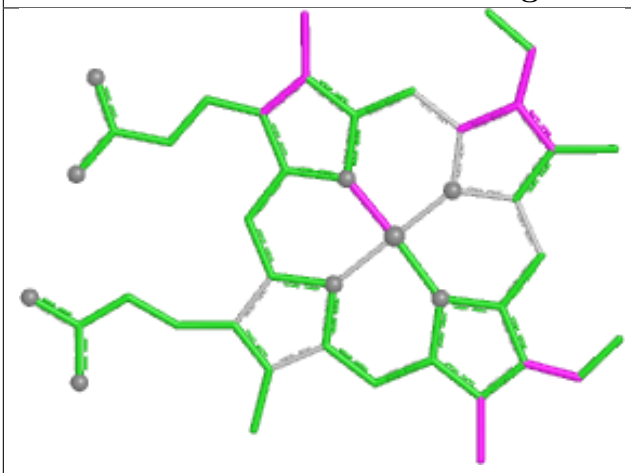

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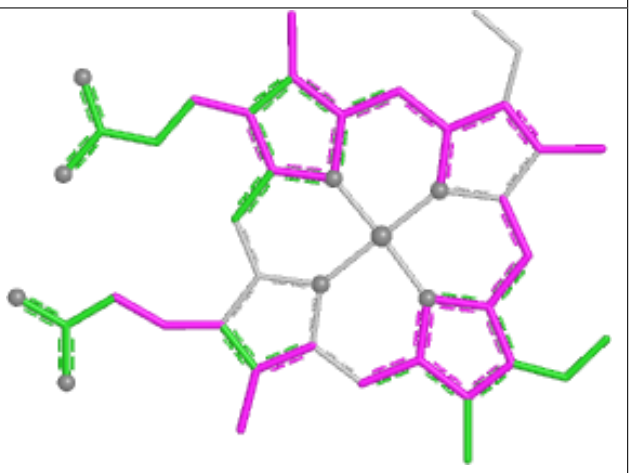

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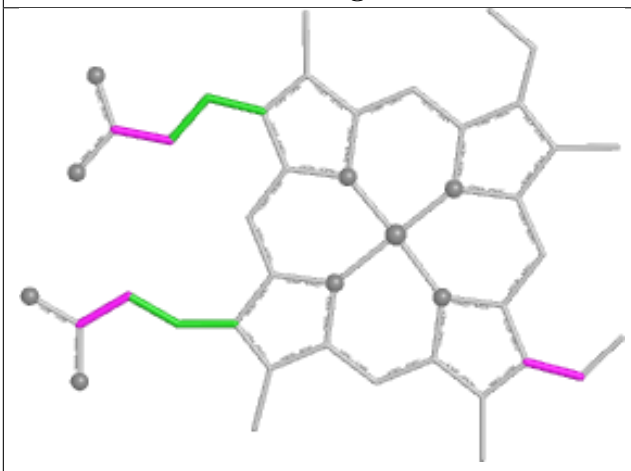

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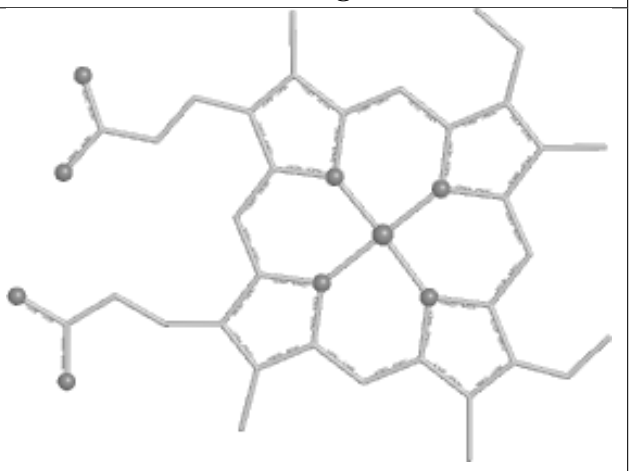

Rings

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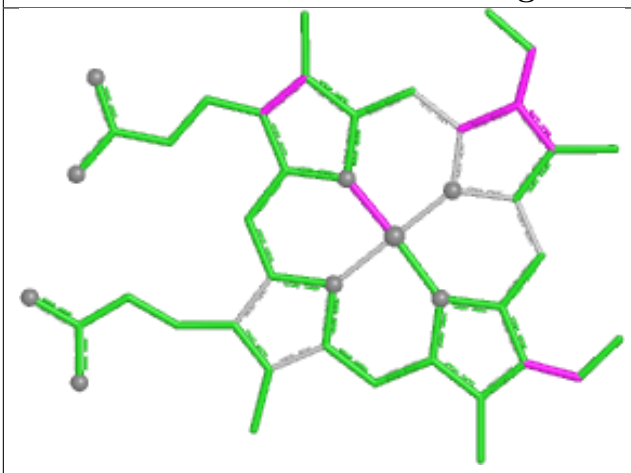

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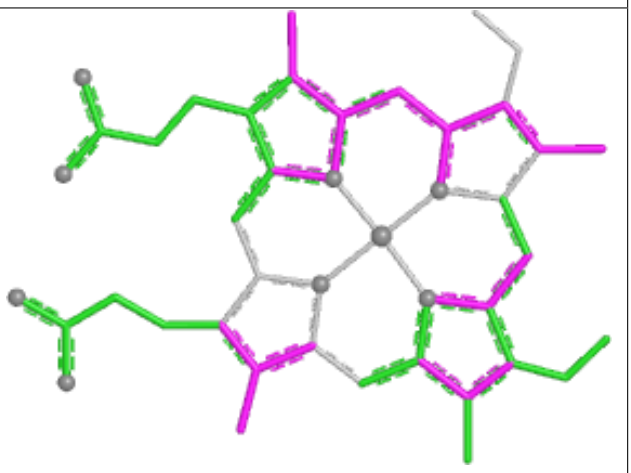

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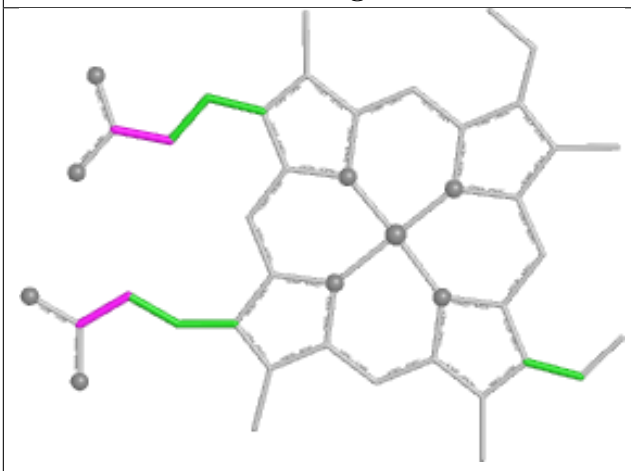

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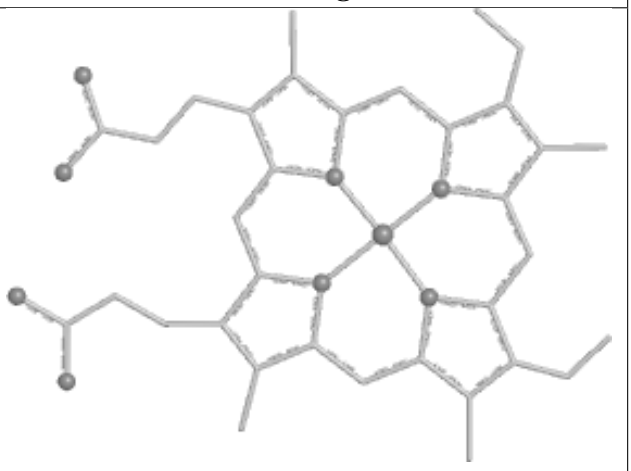
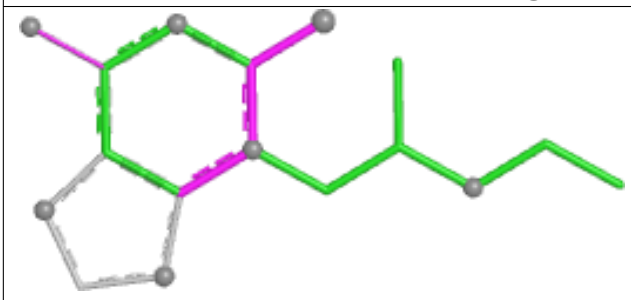


Rings

Ligand 0KY C 601



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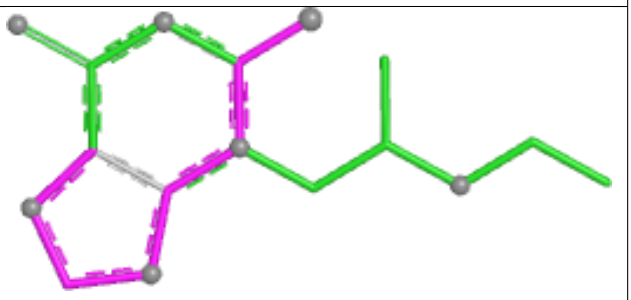

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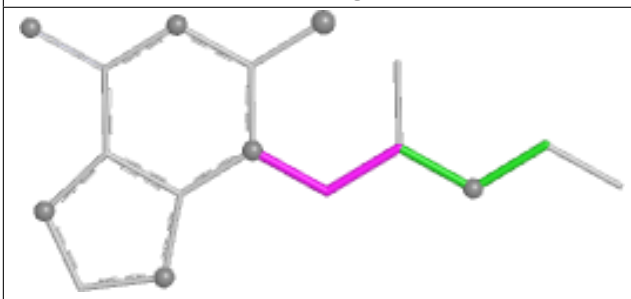

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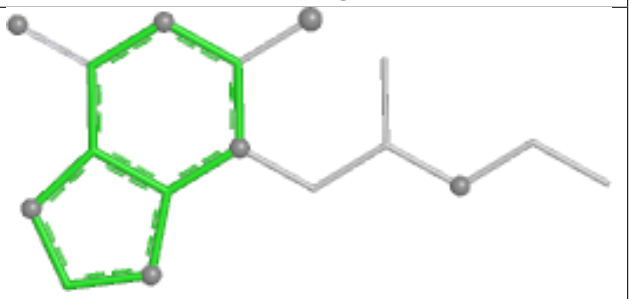

Rings

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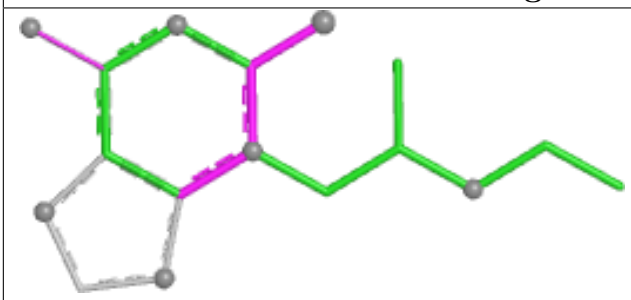

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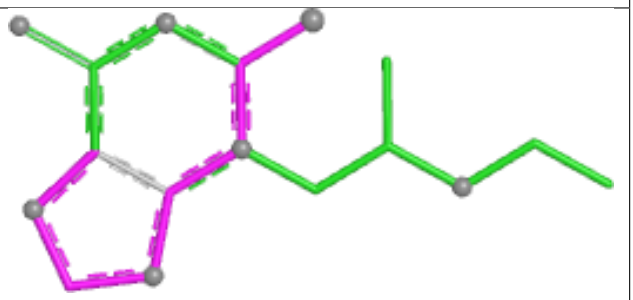

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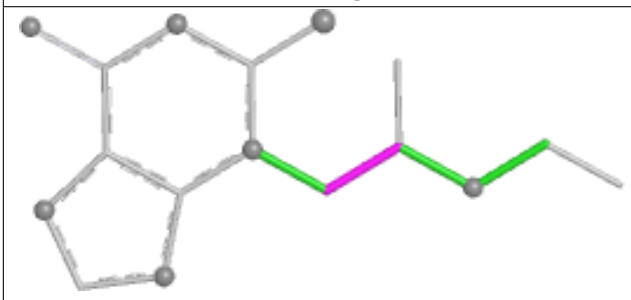

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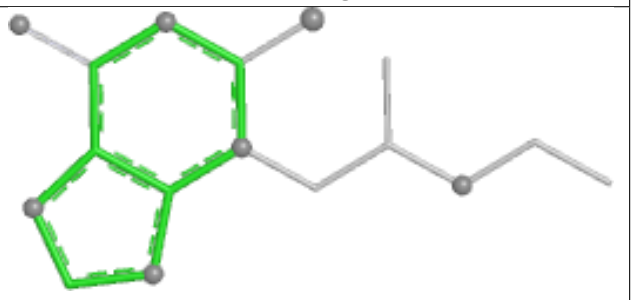
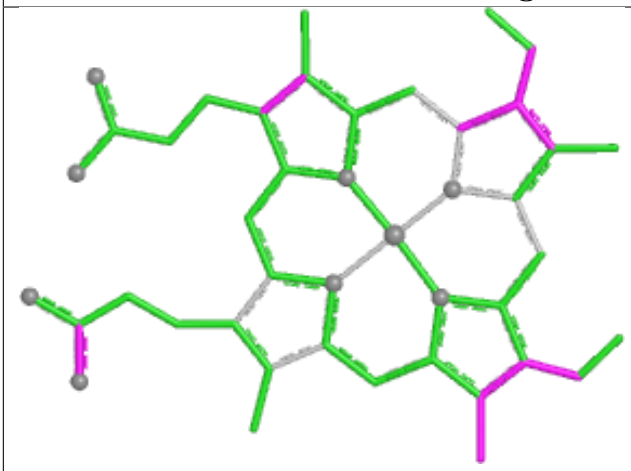


Rings

Ligand HEM G 601



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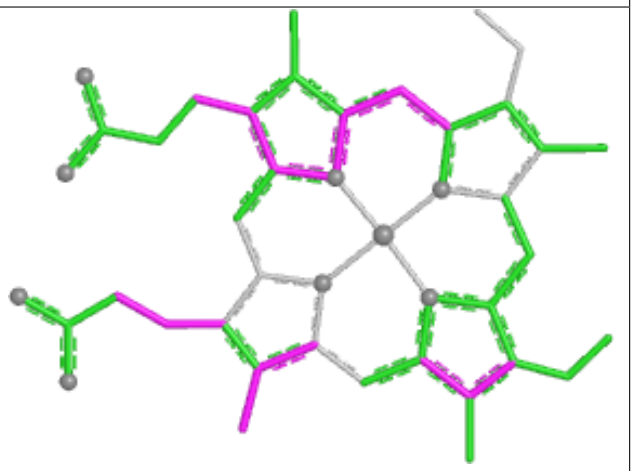

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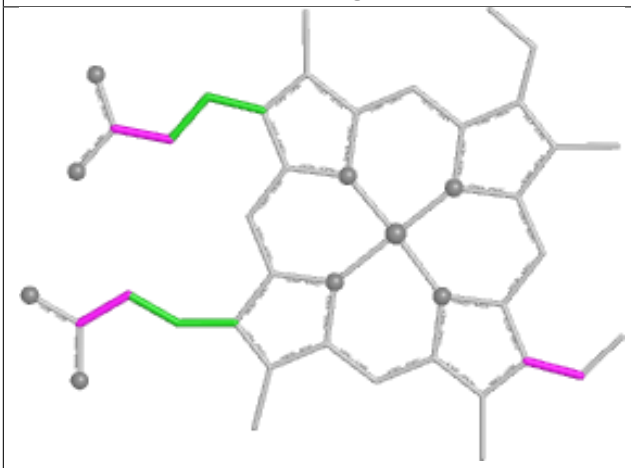

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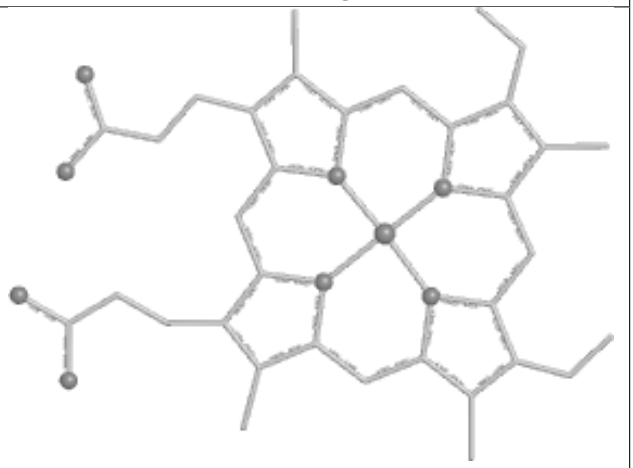
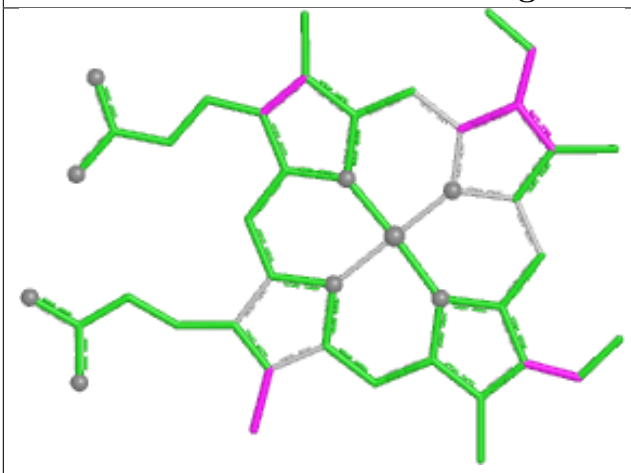


Rings

Ligand HEM O 601



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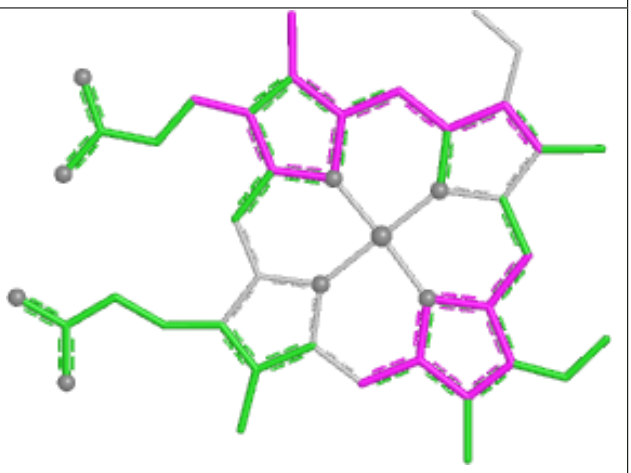
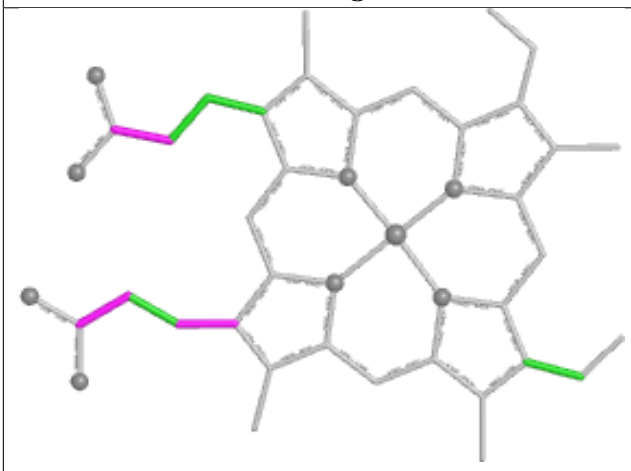


Bond angles



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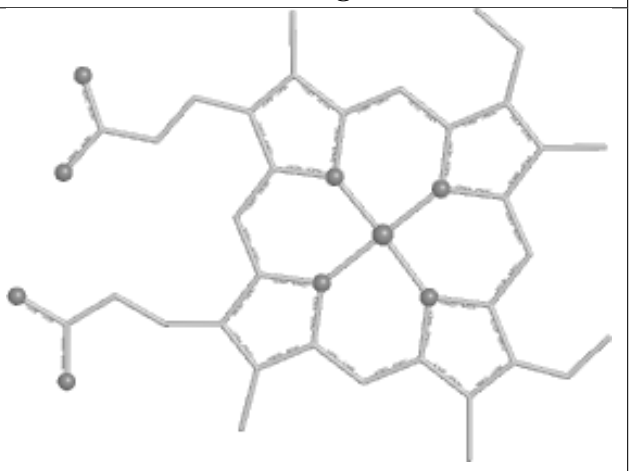
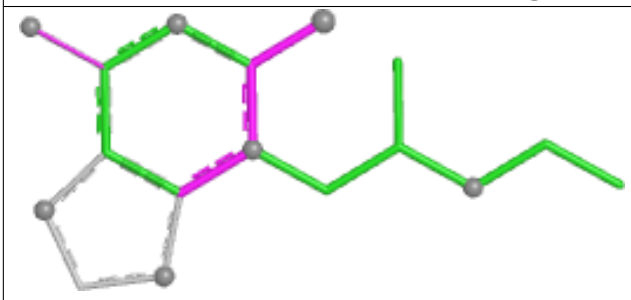


Rings

Ligand 0KY P 604



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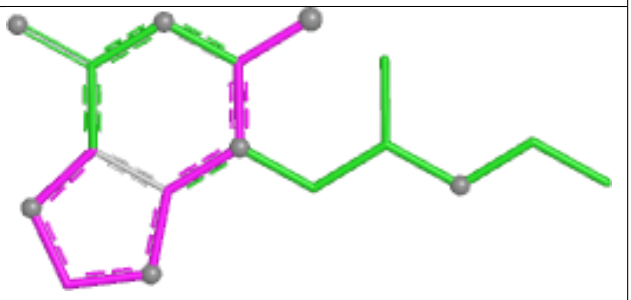
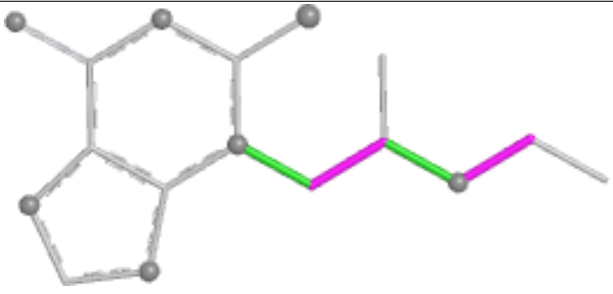
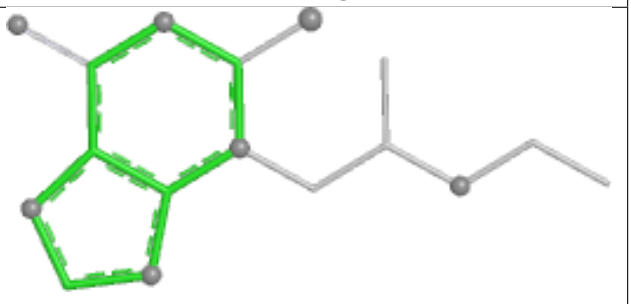


Bond angles

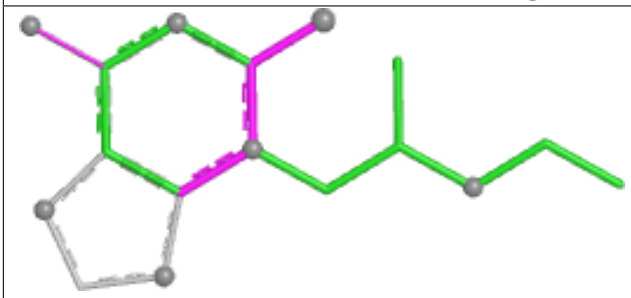


Torsions



Rings

Ligand 0KY K 602



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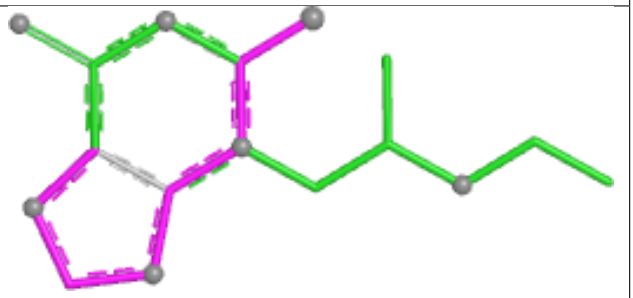
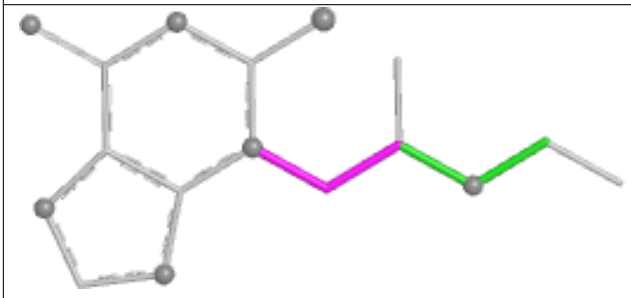
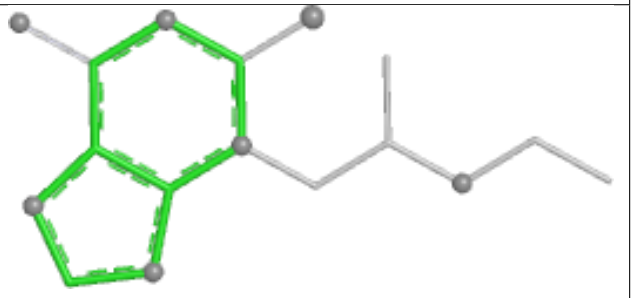


Bond angles

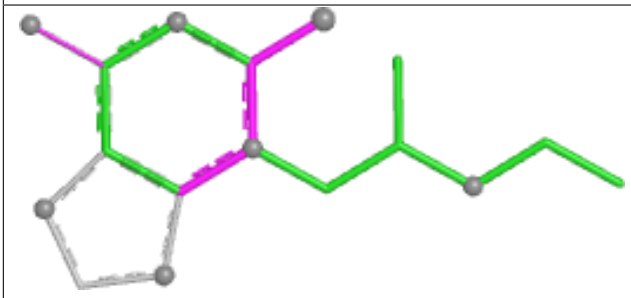


Torsions

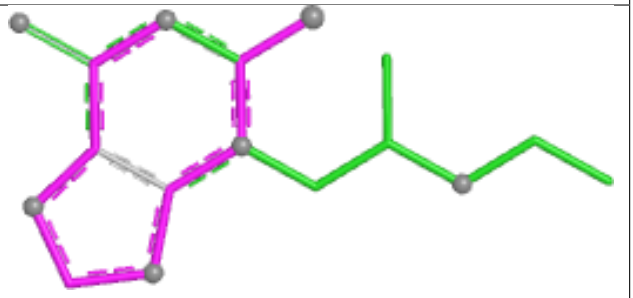


Rings

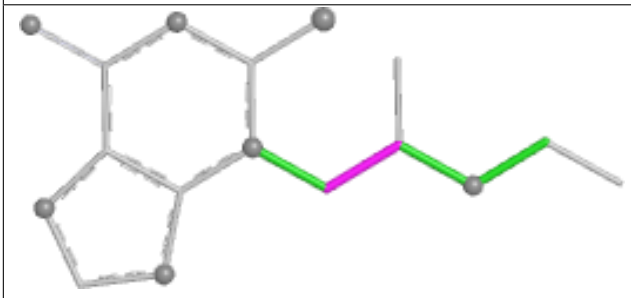
Ligand 0KY L 602



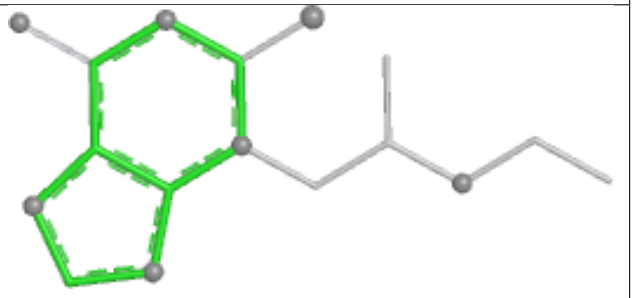
Bond lengths



Bond angles

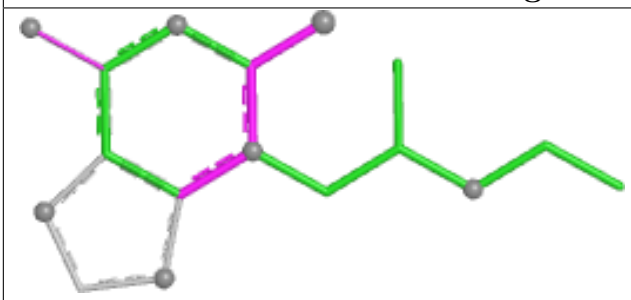


Torsions

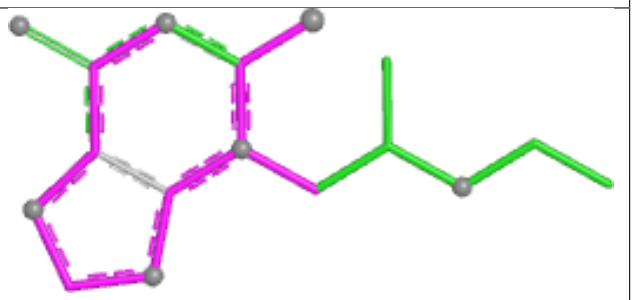


Rings

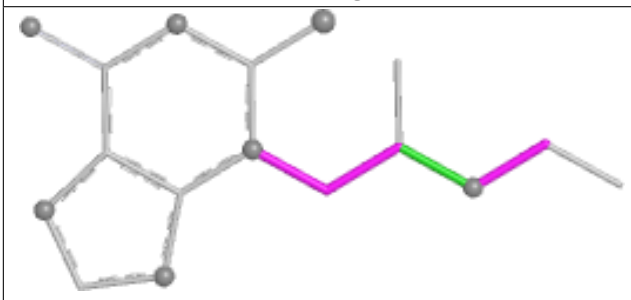
Ligand 0KY H 605



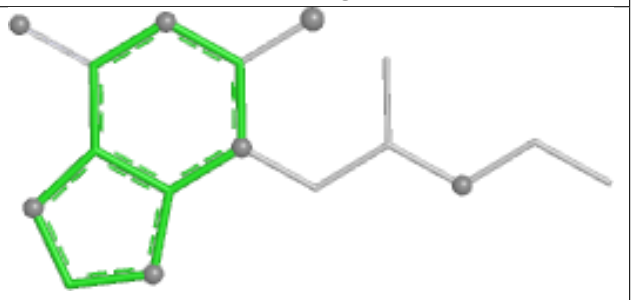
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	104/104 (100%)	-1.68	0	100	100	12, 18, 40, 58	0
1	B	104/104 (100%)	-1.63	0	100	100	14, 24, 40, 53	0
1	E	104/104 (100%)	-1.62	0	100	100	15, 23, 47, 67	0
1	F	104/104 (100%)	-1.55	0	100	100	16, 30, 51, 56	0
1	I	104/104 (100%)	-1.61	0	100	100	16, 24, 44, 65	0
1	J	104/104 (100%)	-1.57	0	100	100	16, 26, 45, 52	0
1	M	104/104 (100%)	-1.55	0	100	100	16, 26, 49, 67	0
1	N	104/104 (100%)	-1.50	0	100	100	14, 32, 56, 63	1 (0%)
2	C	464/466 (99%)	-1.69	0	100	100	11, 20, 36, 58	1 (0%)
2	D	465/466 (99%)	-1.62	0	100	100	13, 26, 45, 63	0
2	G	464/466 (99%)	-1.60	0	100	100	12, 29, 52, 67	0
2	H	465/466 (99%)	-1.51	0	100	100	17, 33, 54, 72	0
2	K	464/466 (99%)	-1.57	0	100	100	12, 29, 54, 73	0
2	L	465/466 (99%)	-1.58	0	100	100	15, 27, 44, 65	0
2	O	465/466 (99%)	-1.56	0	100	100	17, 30, 52, 67	0
2	P	465/466 (99%)	-1.51	0	100	100	17, 31, 59, 77	0
All	All	4549/4560 (99%)	-1.58	0	100	100	11, 28, 51, 77	2 (0%)

There are no RSRZ outliers to report.

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

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, 95^{th} 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
2	CSO	C	150	7/8	1.00	0.02	14,15,22,24	0
2	CSO	D	150	7/8	1.00	0.02	17,19,23,24	0
2	CSO	G	150	7/8	1.00	0.02	15,16,25,26	0
2	CSO	H	150	7/8	1.00	0.02	21,24,29,34	0
2	CSO	K	150	7/8	1.00	0.02	22,24,26,30	0
2	CSO	L	150	7/8	1.00	0.02	22,24,25,30	0
2	CSO	O	150	7/8	1.00	0.02	19,20,28,28	0
2	CSO	P	150	7/8	1.00	0.02	26,29,33,36	0

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, 95^{th} 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	Q	4	11/12	0.98	0.04	47,52,54,56	0
3	MAN	R	4	11/12	0.98	0.04	44,49,54,54	0
3	MAN	S	4	11/12	0.98	0.04	58,63,67,67	0
3	FUC	S	6	10/11	0.98	0.04	29,36,39,42	0
3	MAN	T	4	11/12	0.98	0.04	46,51,53,54	0
3	MAN	V	4	11/12	0.98	0.04	39,46,48,49	0
4	MAN	Y	4	11/12	0.98	0.04	43,45,47,51	0
3	NAG	Q	2	14/15	0.99	0.02	14,22,27,28	0
3	MAN	R	5	11/12	0.99	0.03	23,28,32,33	0
3	FUC	R	6	10/11	0.99	0.03	18,22,26,27	0
3	NAG	S	1	14/15	0.99	0.03	29,34,41,42	0
3	NAG	S	2	14/15	0.99	0.02	29,31,35,37	0
3	BMA	S	3	11/12	0.99	0.03	36,42,46,49	0
3	BMA	Q	3	11/12	0.99	0.03	24,28,32,36	0
3	MAN	S	5	11/12	0.99	0.04	34,38,39,39	0
3	NAG	Q	1	14/15	0.99	0.02	17,21,28,30	0
3	NAG	T	1	14/15	0.99	0.03	19,24,31,34	0
3	NAG	T	2	14/15	0.99	0.03	21,25,27,27	0
3	MAN	Q	5	11/12	0.99	0.03	24,29,31,31	0
3	MAN	T	5	11/12	0.99	0.03	28,33,37,40	0
3	FUC	T	6	10/11	0.99	0.03	24,27,31,38	0
3	NAG	U	2	14/15	0.99	0.02	18,23,27,27	0
3	BMA	U	3	11/12	0.99	0.03	22,25,31,37	0
3	MAN	U	4	11/12	0.99	0.04	45,53,54,57	0
3	MAN	U	5	11/12	0.99	0.03	24,30,34,34	0
3	FUC	U	6	10/11	0.99	0.03	28,31,34,35	0

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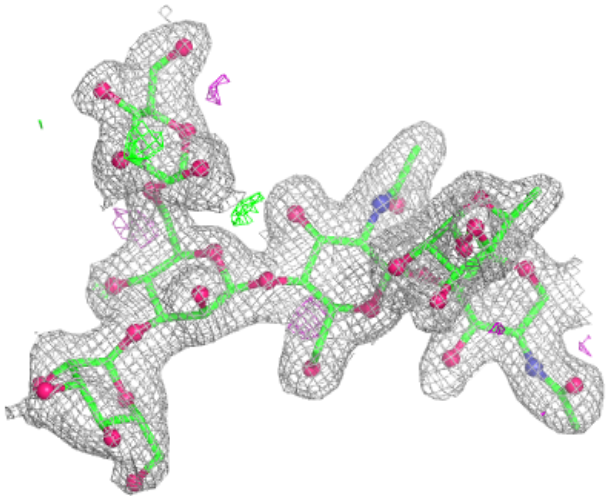
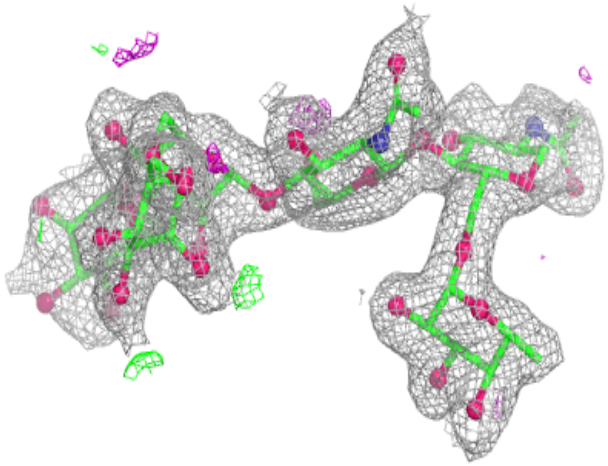
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	V	1	14/15	0.99	0.02	16,21,28,30	0
3	NAG	V	2	14/15	0.99	0.02	15,17,20,22	0
3	BMA	V	3	11/12	0.99	0.03	21,26,31,36	0
3	FUC	Q	6	10/11	0.99	0.03	23,27,29,32	0
3	MAN	V	5	11/12	0.99	0.03	26,30,33,33	0
3	FUC	V	6	10/11	0.99	0.03	26,29,30,31	0
3	NAG	W	1	14/15	0.99	0.03	28,33,41,45	0
3	NAG	W	2	14/15	0.99	0.02	22,30,38,42	0
3	BMA	W	3	11/12	0.99	0.02	35,37,40,44	0
3	MAN	W	4	11/12	0.99	0.03	51,55,64,70	0
3	MAN	W	5	11/12	0.99	0.03	29,35,37,38	0
3	FUC	W	6	10/11	0.99	0.03	36,37,39,40	0
3	NAG	X	1	14/15	0.99	0.03	25,28,39,40	0
3	BMA	X	3	11/12	0.99	0.02	24,31,36,41	0
3	MAN	X	4	11/12	0.99	0.03	44,54,61,62	0
3	MAN	X	5	11/12	0.99	0.03	28,34,36,37	0
3	FUC	X	6	10/11	0.99	0.03	28,30,31,33	0
4	NAG	Y	1	14/15	0.99	0.02	23,27,30,30	0
4	NAG	Y	2	14/15	0.99	0.04	28,30,36,37	0
4	BMA	Y	3	11/12	0.99	0.02	28,33,39,46	0
3	BMA	R	3	11/12	0.99	0.02	18,22,26,31	0
4	MAN	Y	5	11/12	0.99	0.04	46,52,57,57	0
3	NAG	X	2	14/15	1.00	0.02	19,25,28,30	0
3	BMA	T	3	11/12	1.00	0.02	25,27,33,38	0
3	NAG	U	1	14/15	1.00	0.02	19,25,32,33	0
3	NAG	R	1	14/15	1.00	0.02	15,21,28,32	0
3	NAG	R	2	14/15	1.00	0.02	15,18,22,22	0

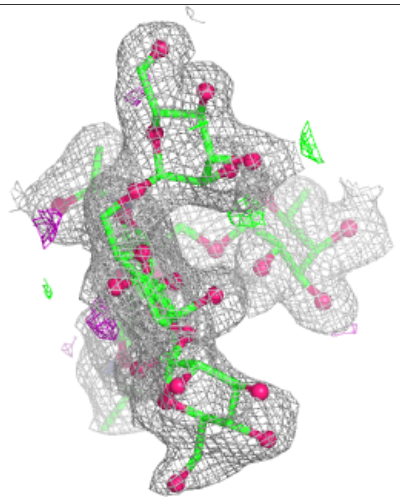
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Q:

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

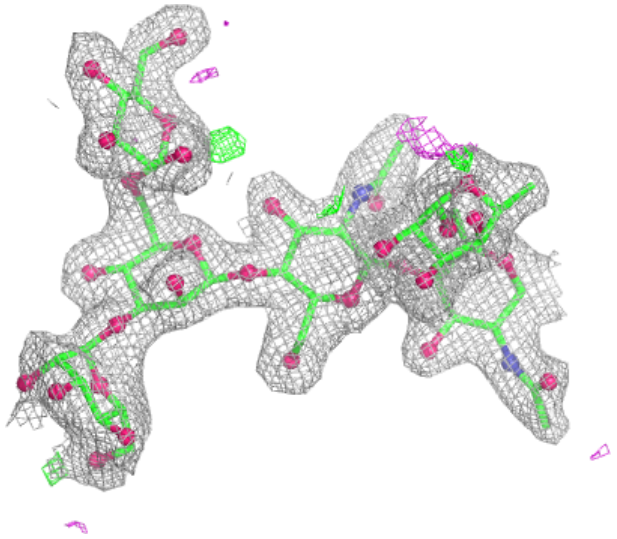


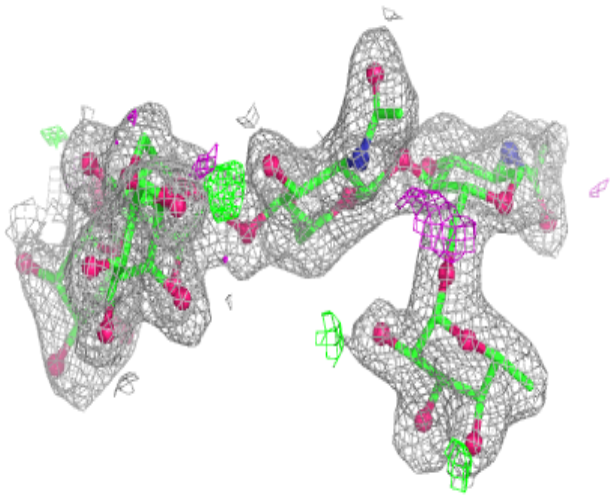


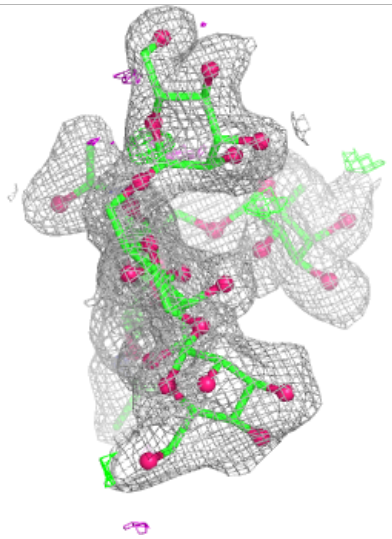


Electron density around Chain R:

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

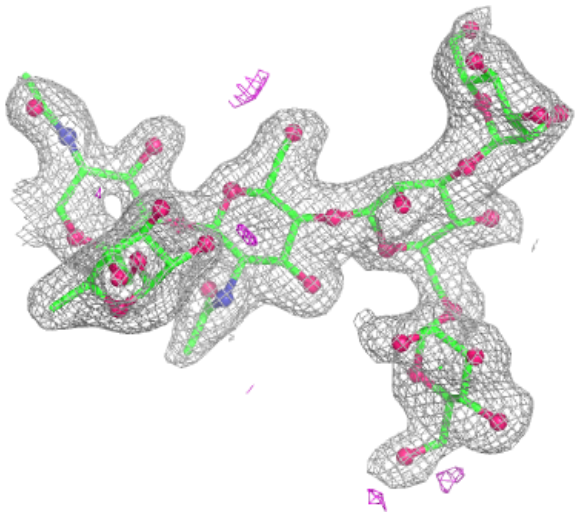


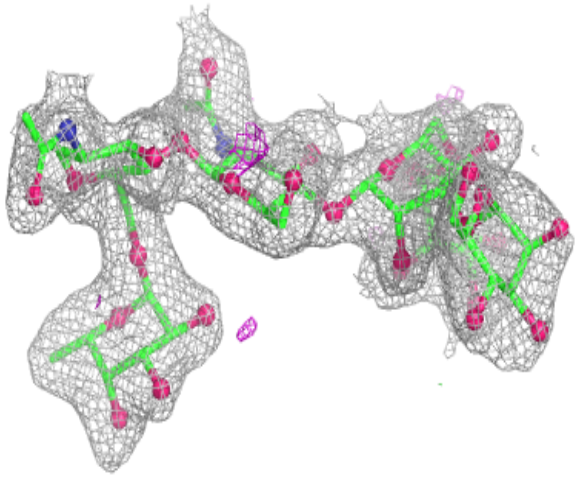


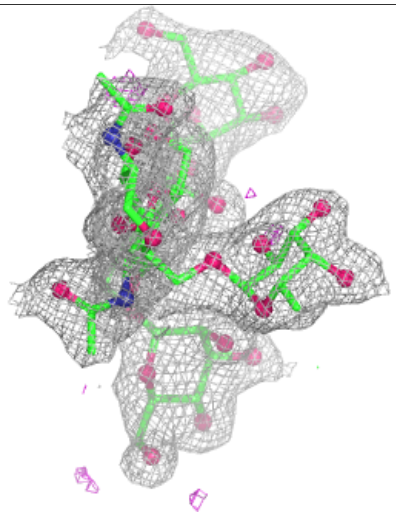


Electron density around Chain S:

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

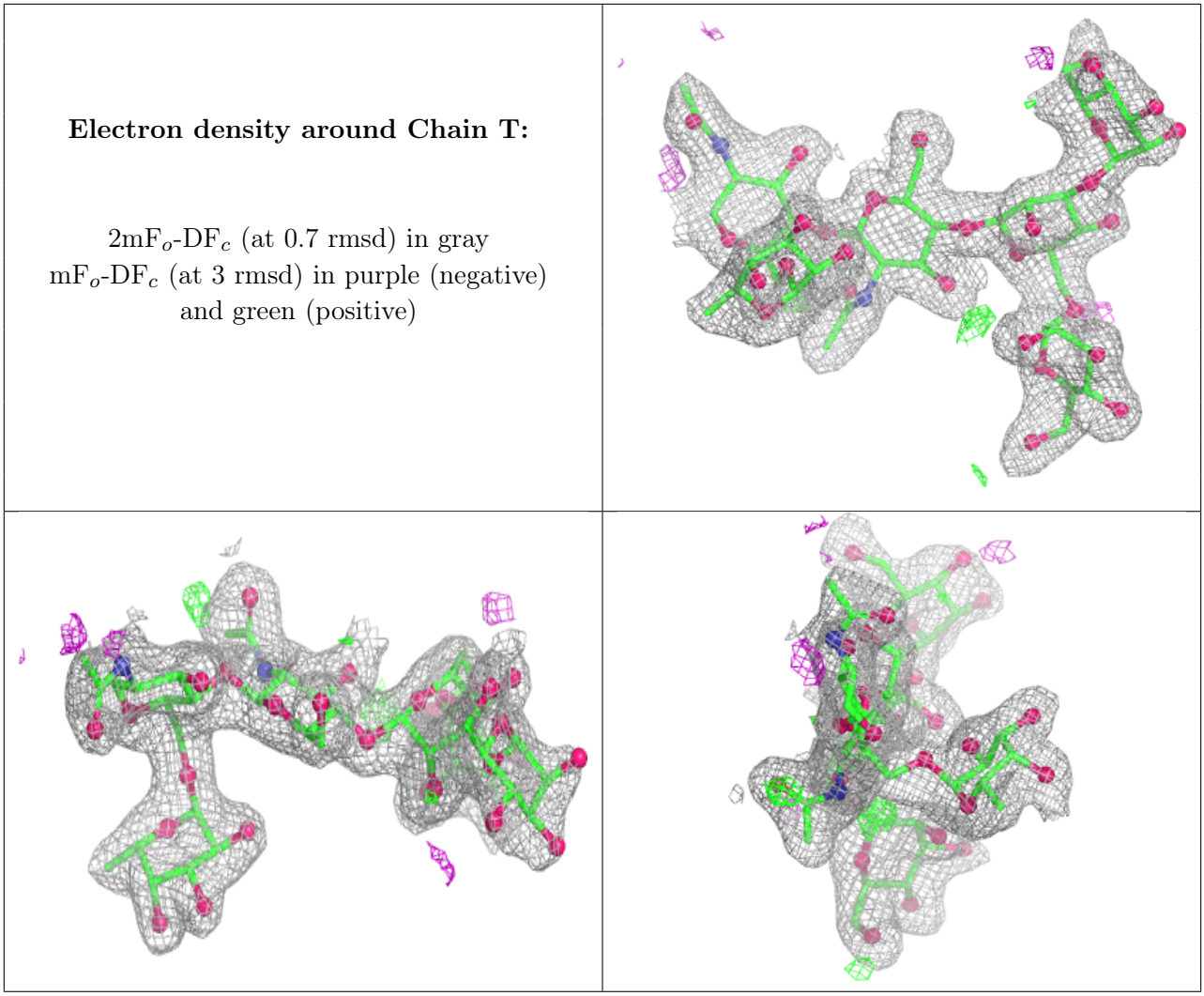






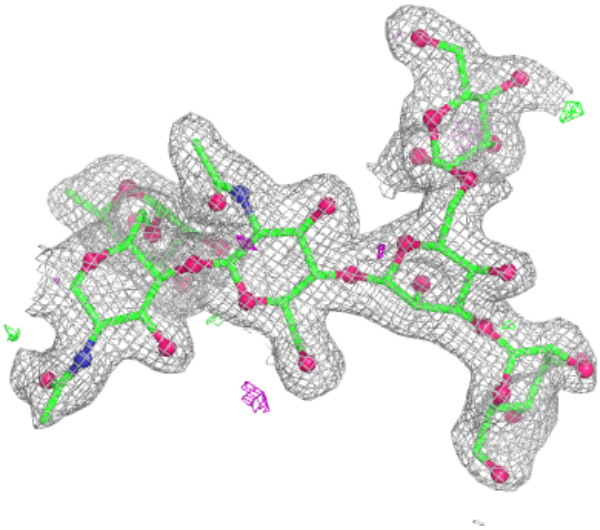
Electron density around Chain T:

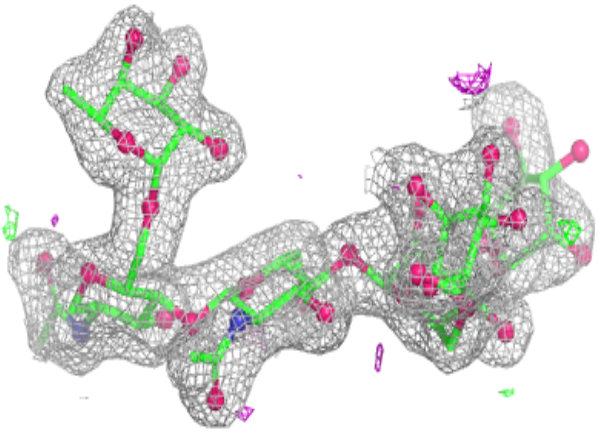
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

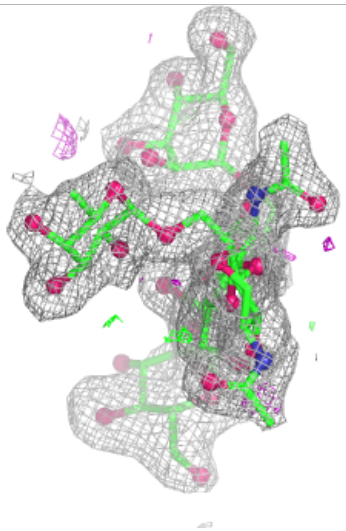


Electron density around Chain U:

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

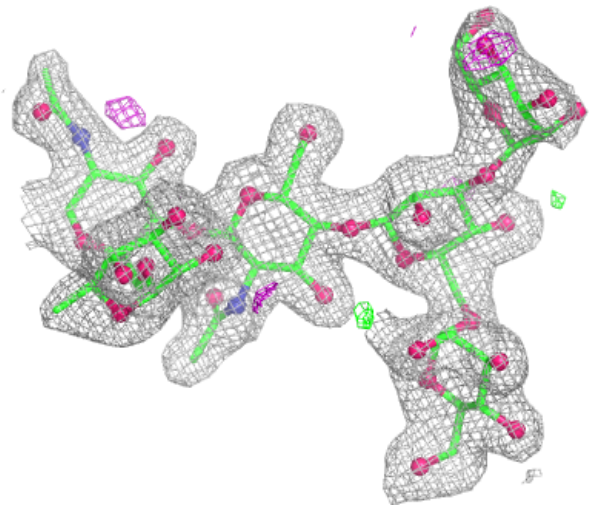


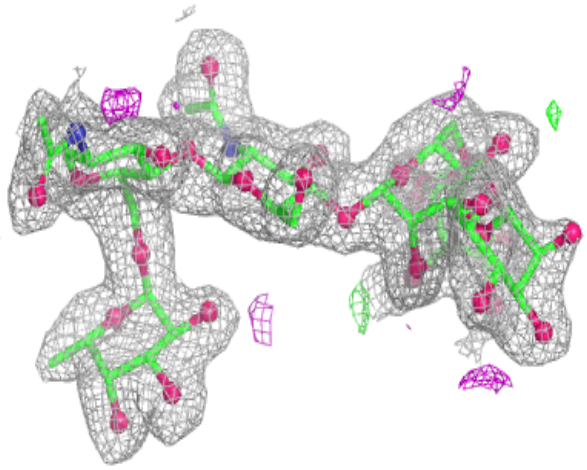


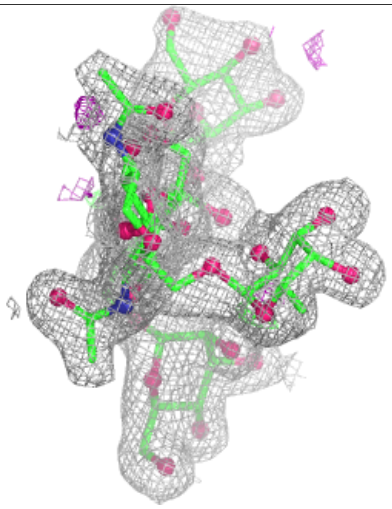


Electron density around Chain V:

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

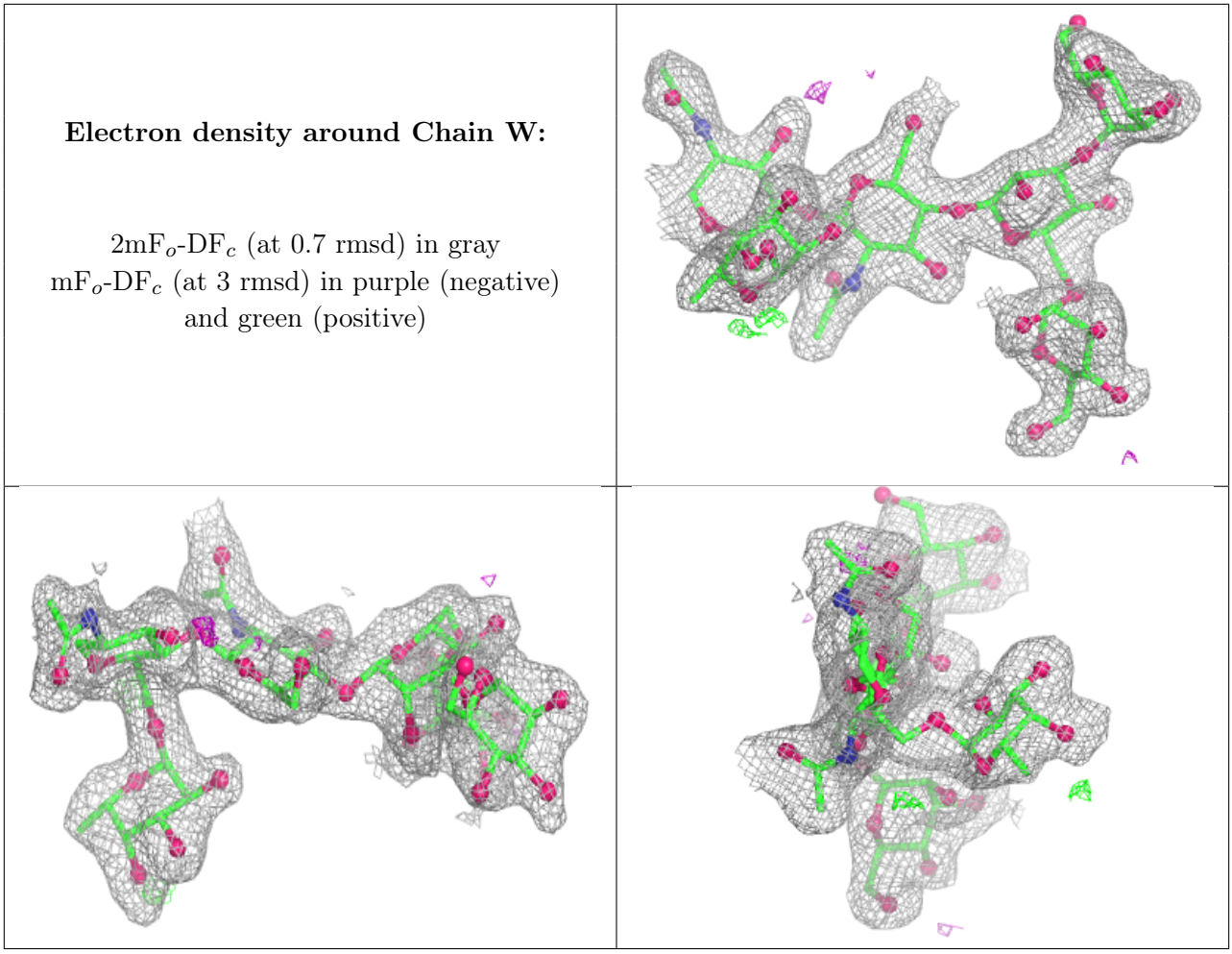






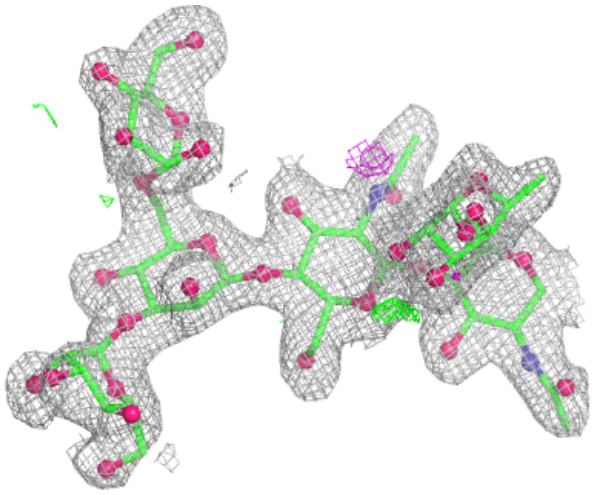
Electron density around Chain W:

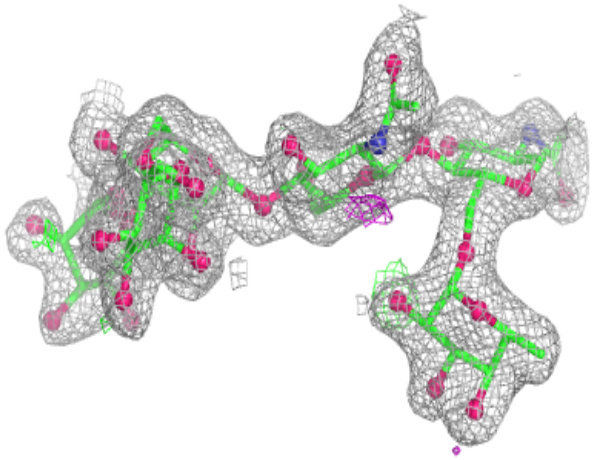
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

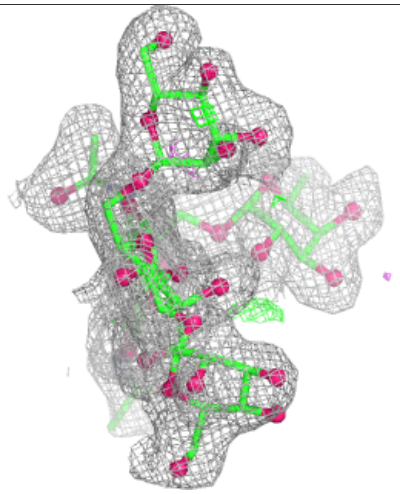


Electron density around Chain X:

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

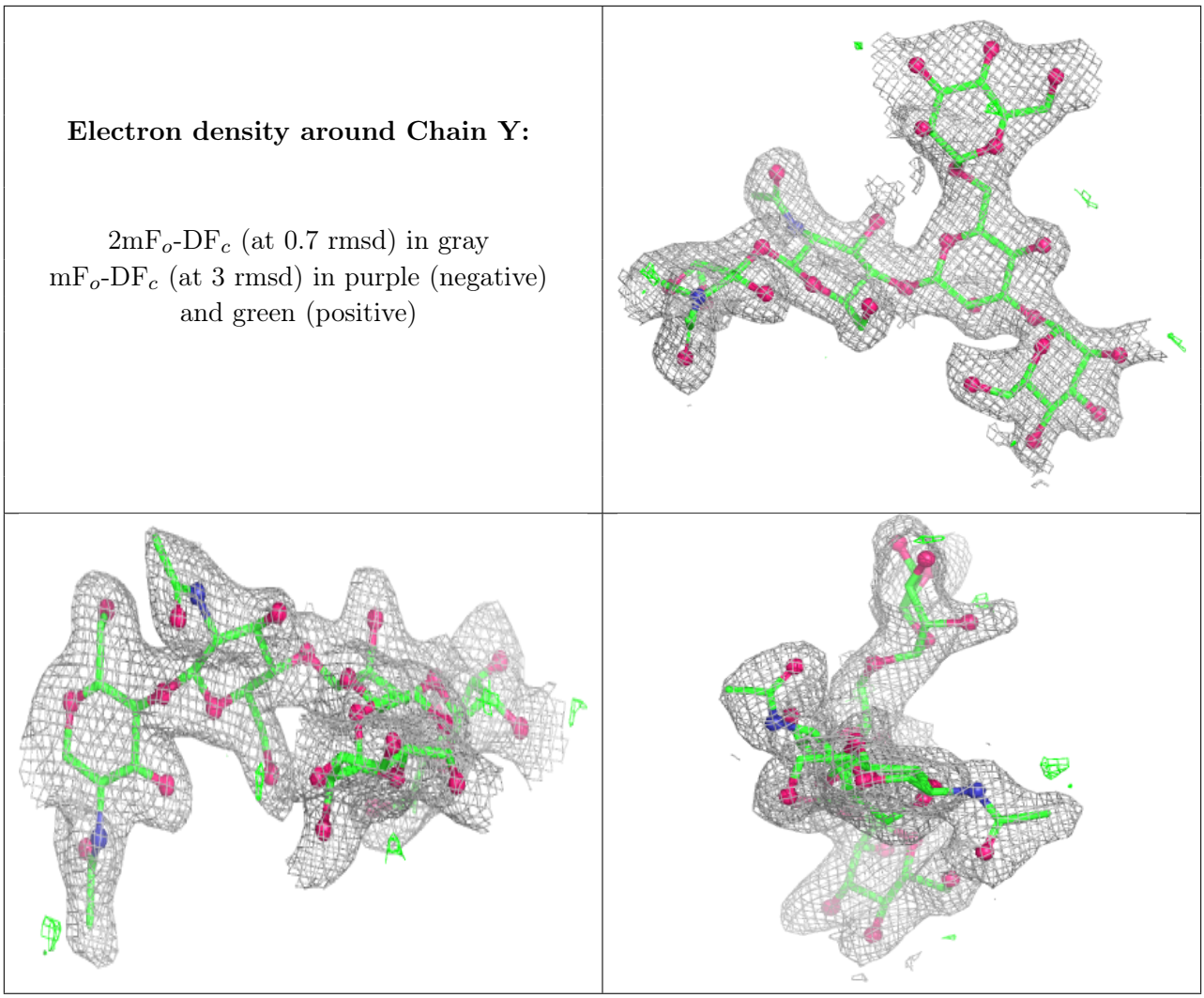






Electron density around Chain Y:

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



6.4 Ligands

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, 95^{th} 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
8	NAG	O	603	14/15	0.97	0.06	71,75,81,84	0
6	0KY	G	605	17/17	0.98	0.05	38,53,62,62	0
6	0KY	H	605	17/17	0.98	0.06	52,67,75,75	0
6	0KY	K	602	17/17	0.98	0.06	43,59,63,64	0
6	0KY	L	602	17/17	0.98	0.05	50,61,68,68	0
6	0KY	O	605	17/17	0.98	0.06	53,61,70,70	0
6	0KY	P	604	17/17	0.98	0.07	68,78,87,88	0
8	NAG	C	604	14/15	0.98	0.04	54,62,66,66	0
8	NAG	D	604	14/15	0.98	0.04	46,53,55,57	0

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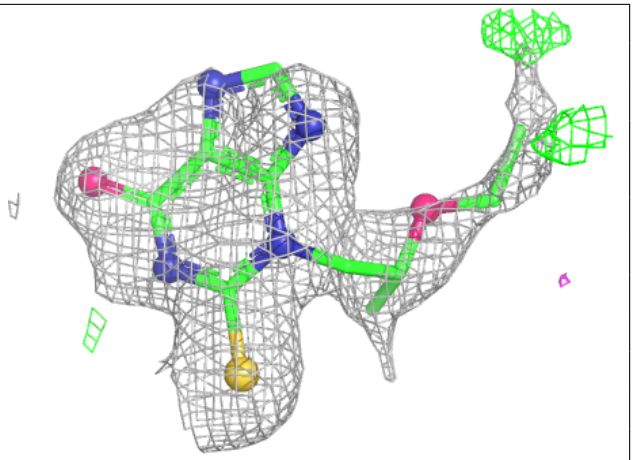
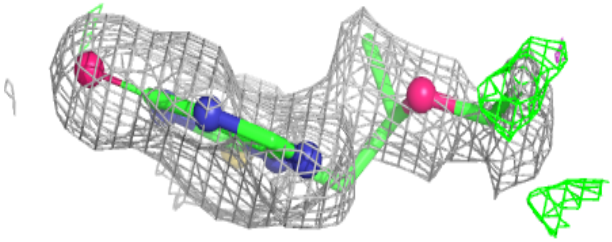
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	G	603	14/15	0.98	0.04	60,67,69,69	0
8	NAG	K	604	14/15	0.98	0.04	49,56,60,61	0
6	0KY	D	602	17/17	0.98	0.06	50,64,66,67	0
8	NAG	P	603	14/15	0.98	0.05	56,61,65,66	0
8	NAG	G	602	14/15	0.99	0.03	32,36,41,43	0
8	NAG	C	603	14/15	0.99	0.03	19,25,29,30	0
8	NAG	H	602	14/15	0.99	0.02	31,37,42,45	0
8	NAG	H	603	14/15	0.99	0.04	62,66,70,72	0
8	NAG	K	603	14/15	0.99	0.04	40,49,53,54	0
6	0KY	C	601	17/17	0.99	0.04	36,43,48,49	0
8	NAG	L	603	14/15	0.99	0.02	27,35,38,39	0
8	NAG	L	604	14/15	0.99	0.04	50,56,59,60	0
8	NAG	O	602	14/15	0.99	0.02	26,28,31,34	0
8	NAG	D	603	14/15	0.99	0.02	24,26,30,36	0
7	HEM	L	601	43/43	0.99	0.03	18,24,29,33	0
5	CL	B	201	1/1	1.00	0.01	14,14,14,14	0
5	CL	E	1601	1/1	1.00	0.01	18,18,18,18	0
5	CL	F	201	1/1	1.00	0.01	25,25,25,25	0
5	CL	I	1601	1/1	1.00	0.01	14,14,14,14	0
5	CL	J	201	1/1	1.00	0.02	20,20,20,20	0
5	CL	M	1601	1/1	1.00	0.01	18,18,18,18	0
5	CL	N	201	1/1	1.00	0.03	21,21,21,21	0
7	HEM	C	602	43/43	1.00	0.02	11,15,20,27	0
7	HEM	D	601	43/43	1.00	0.02	15,21,27,35	0
7	HEM	G	601	43/43	1.00	0.02	13,19,27,28	0
7	HEM	H	601	43/43	1.00	0.03	22,29,33,38	0
7	HEM	K	601	43/43	1.00	0.02	11,20,24,28	0
5	CL	A	1601	1/1	1.00	0.01	16,16,16,16	0
7	HEM	O	601	43/43	1.00	0.02	17,25,28,29	0
7	HEM	P	601	43/43	1.00	0.03	21,30,36,43	0
9	CA	C	605	1/1	1.00	0.01	14,14,14,14	0
9	CA	D	605	1/1	1.00	0.01	16,16,16,16	0
9	CA	G	604	1/1	1.00	0.01	22,22,22,22	0
9	CA	H	604	1/1	1.00	0.01	19,19,19,19	0
9	CA	K	605	1/1	1.00	0.01	24,24,24,24	0
9	CA	L	605	1/1	1.00	0.01	20,20,20,20	0
9	CA	O	604	1/1	1.00	0.02	21,21,21,21	0
9	CA	P	602	1/1	1.00	0.03	19,19,19,19	0

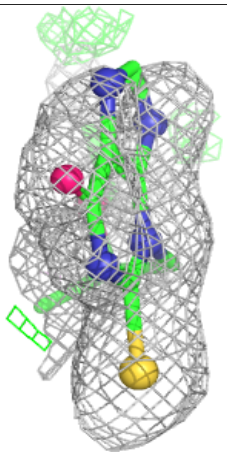
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 0KY G 605:

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

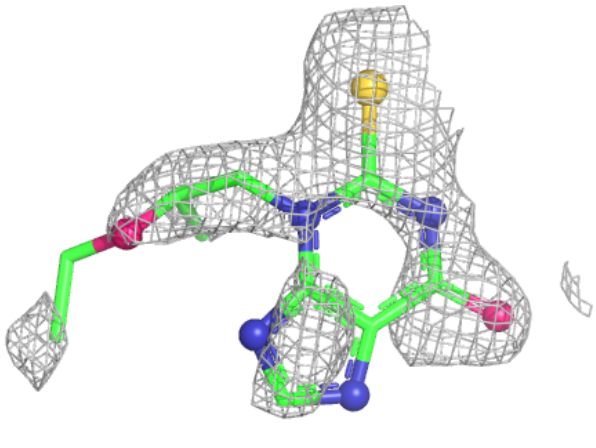


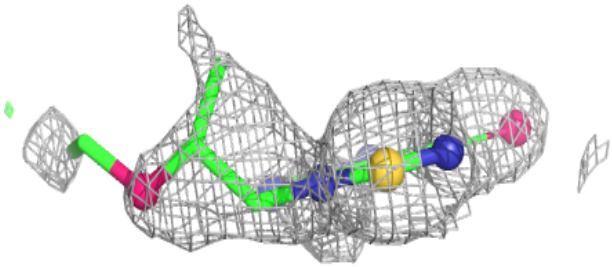


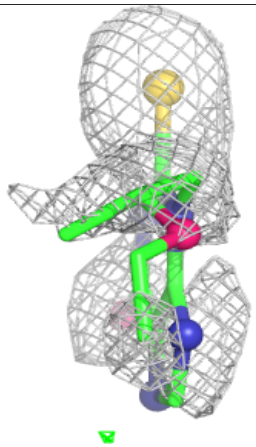


Electron density around 0KY H 605:

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

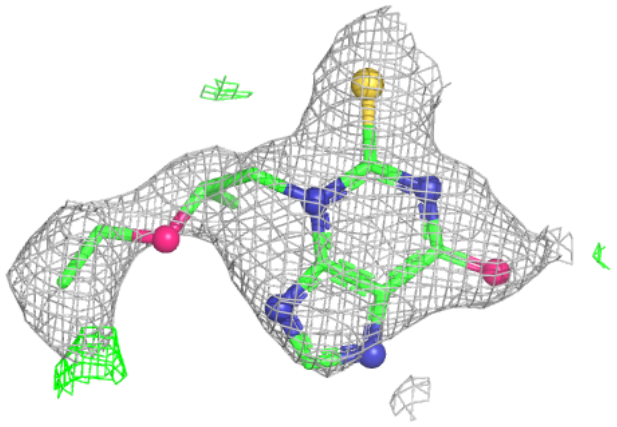


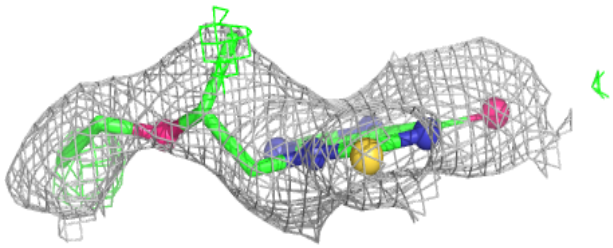


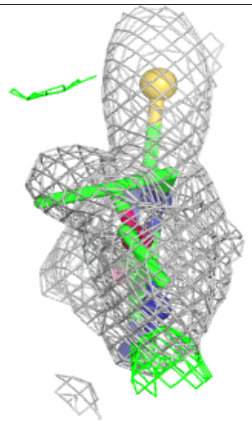


Electron density around 0KY K 602:

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

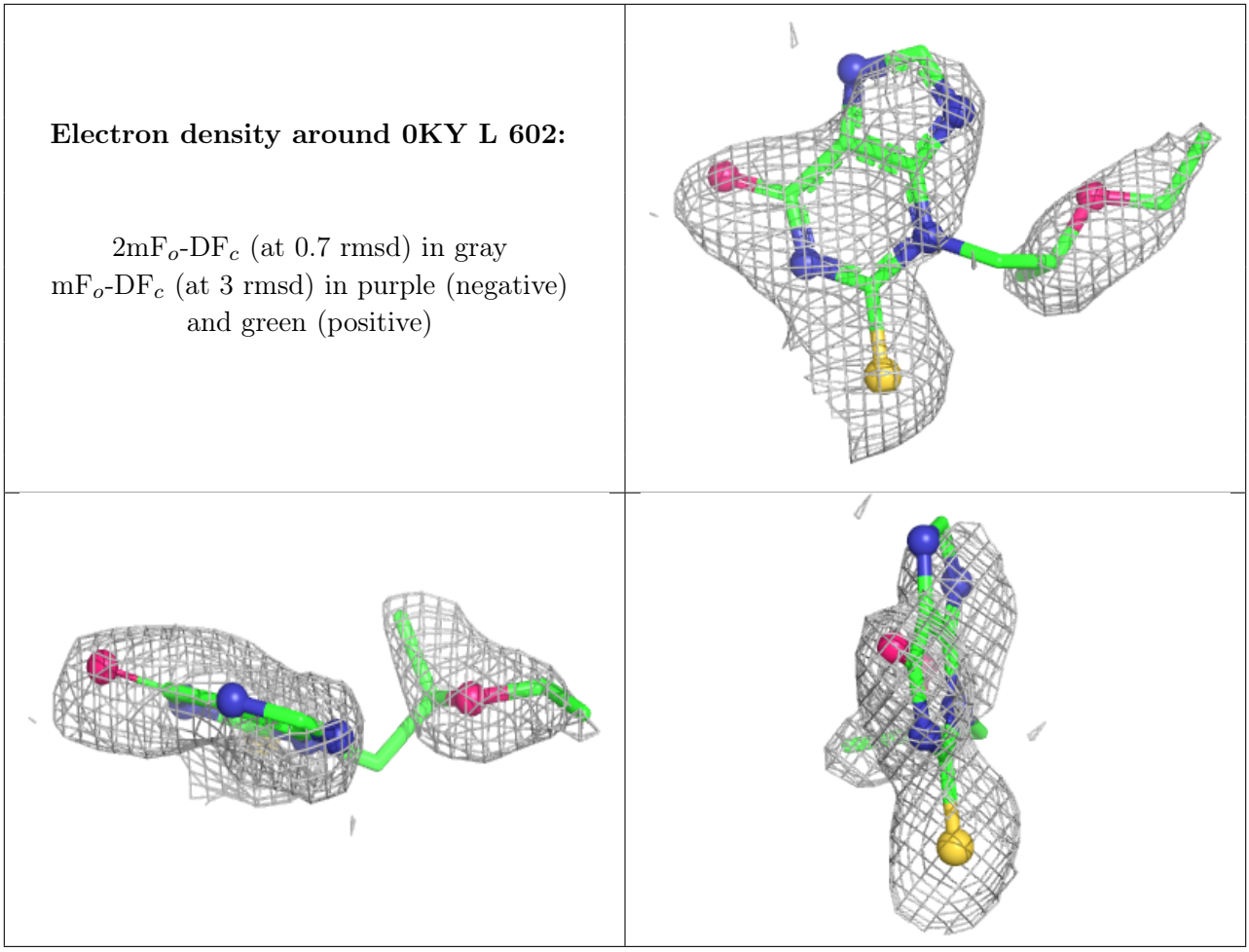






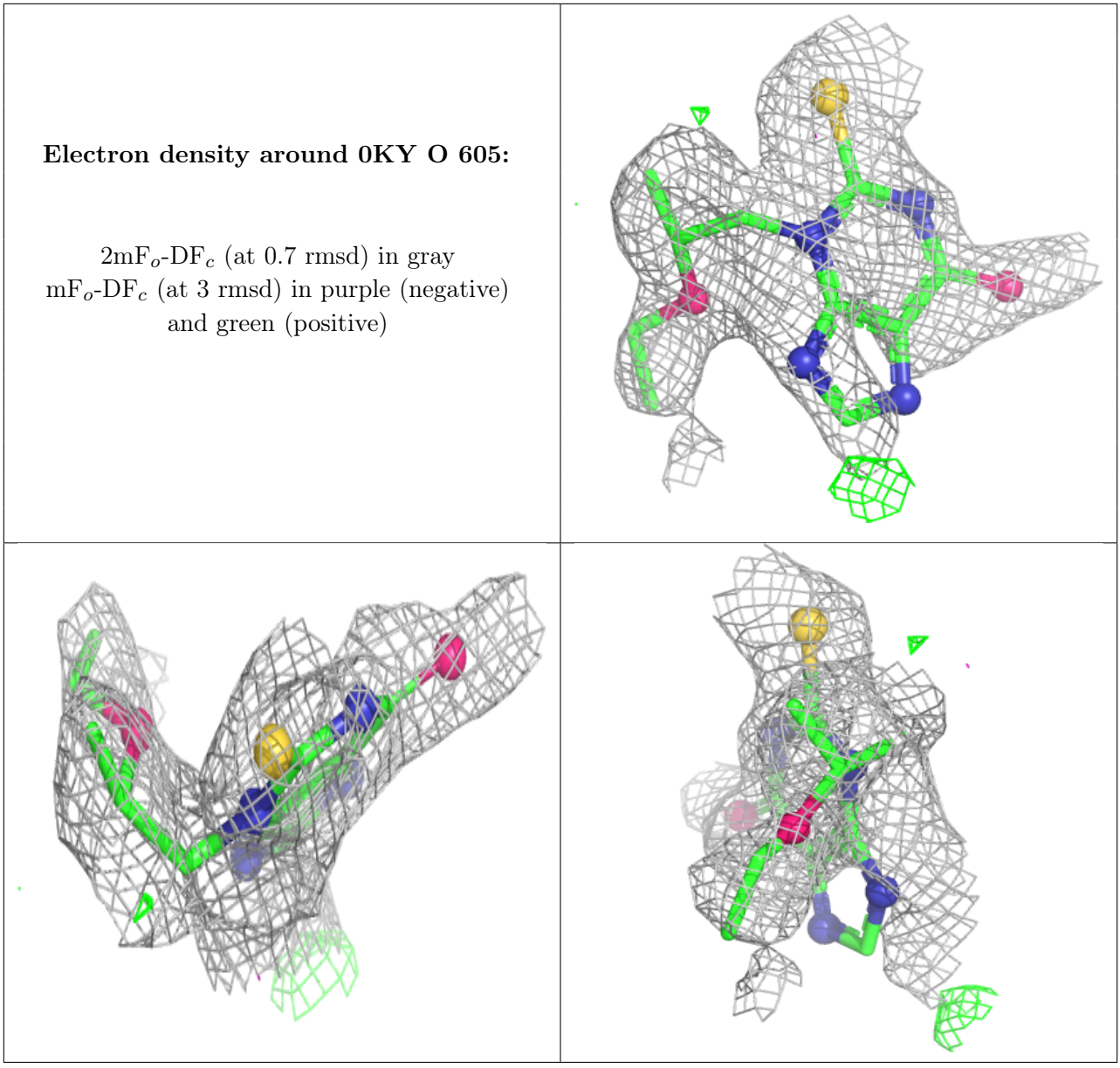
Electron density around 0KY L 602:

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



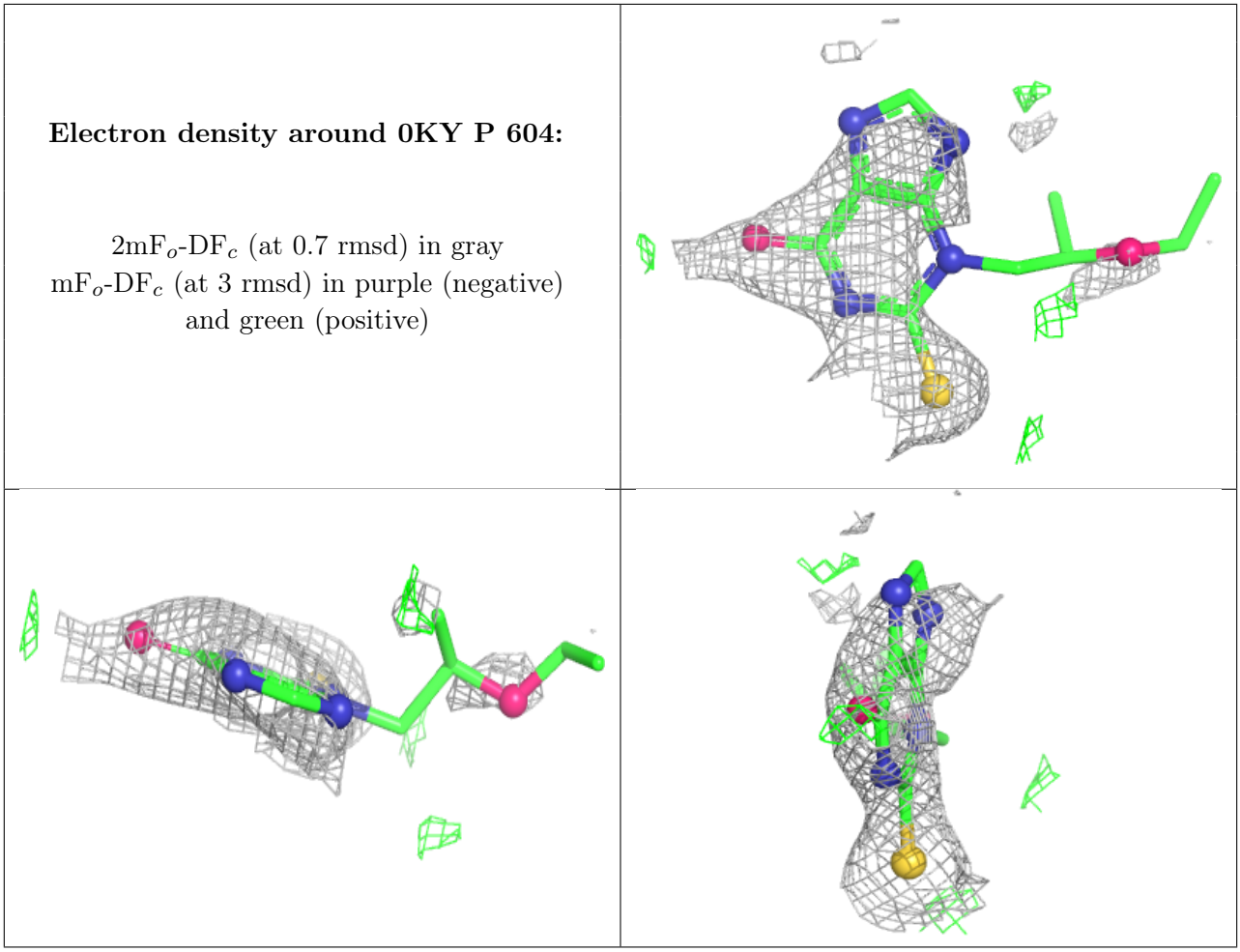
Electron density around 0KY O 605:

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



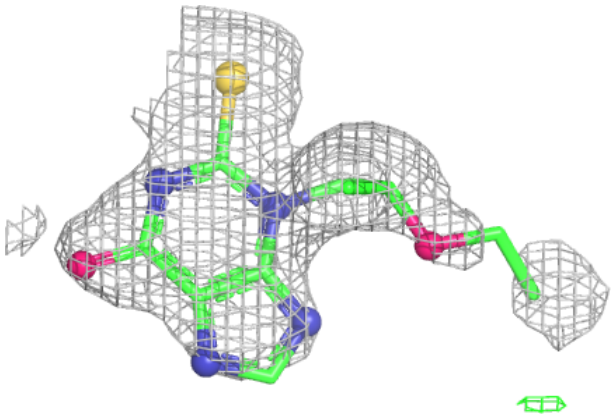
Electron density around 0KY P 604:

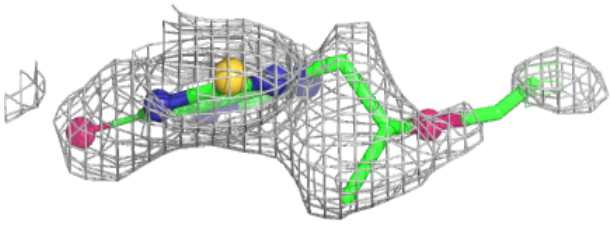
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

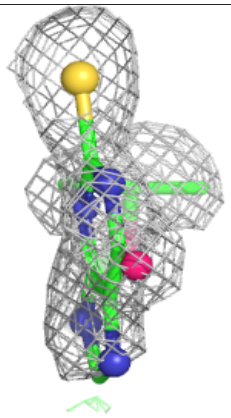


Electron density around 0KY D 602:

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

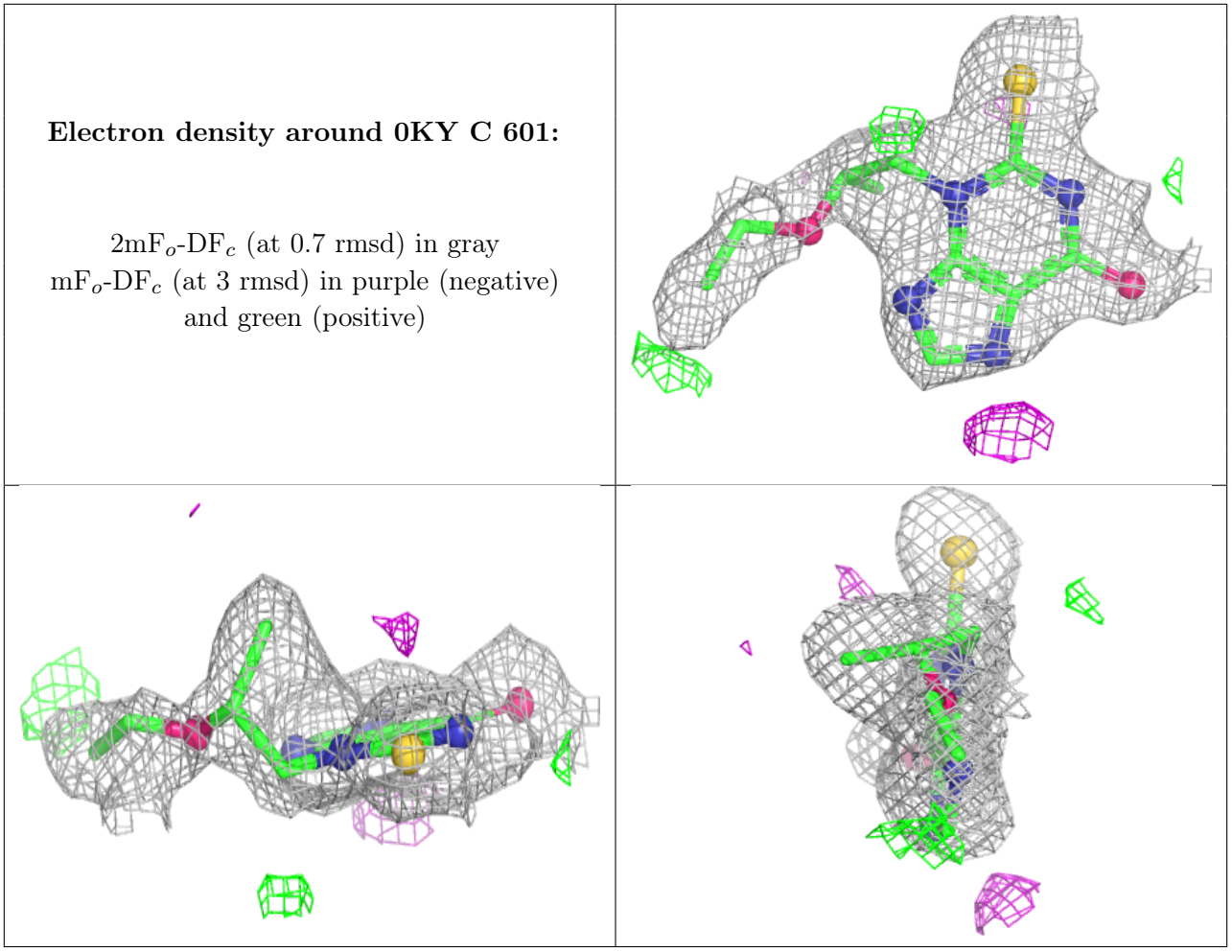






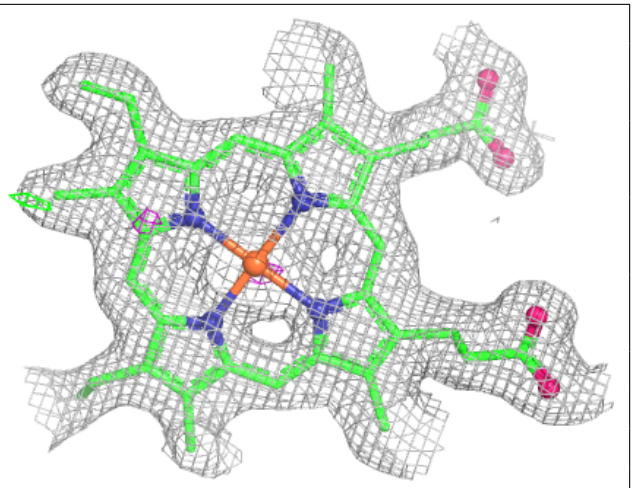
Electron density around 0KY C 601:

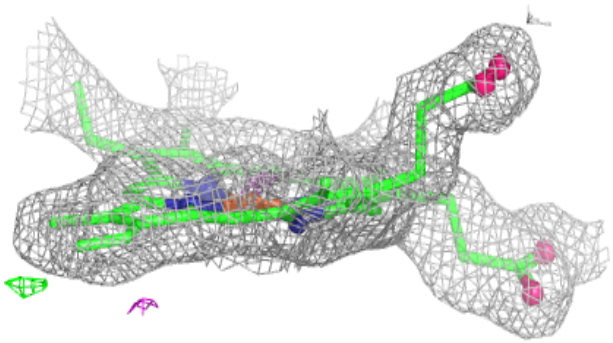
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

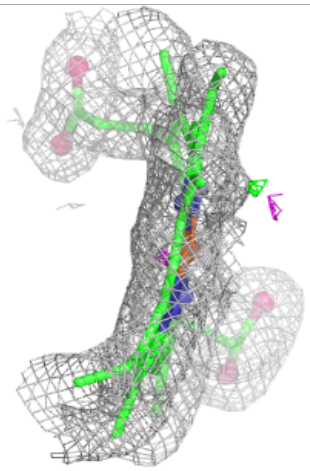


Electron density around HEM L 601:

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

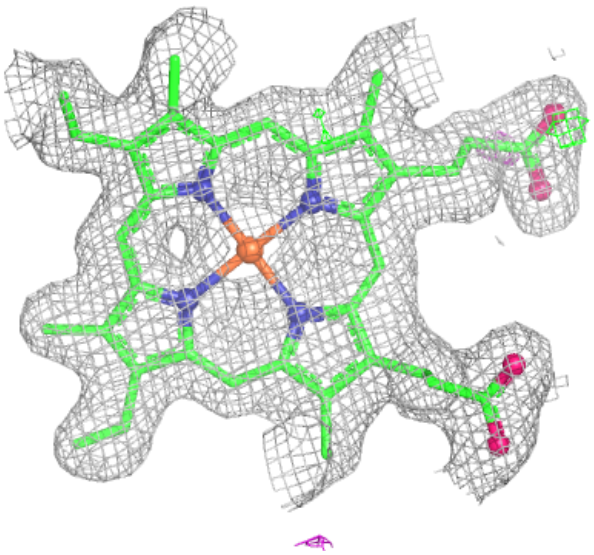


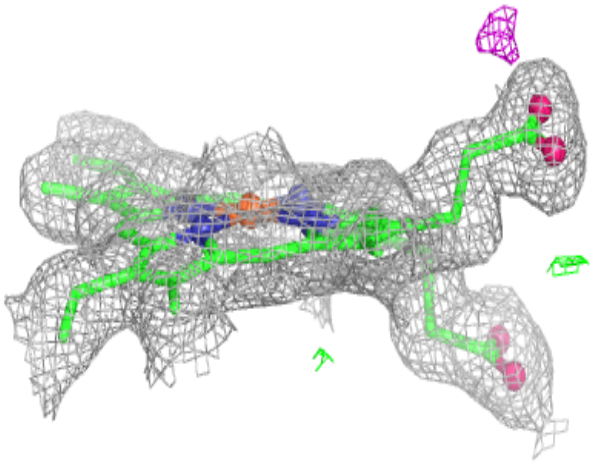


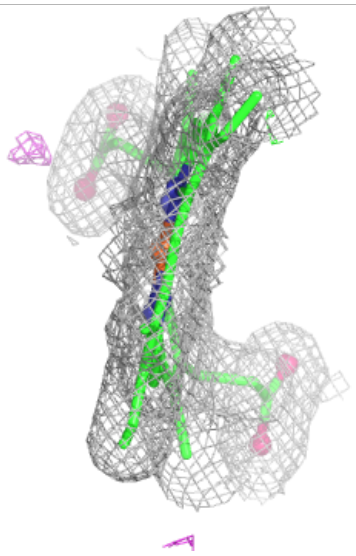


Electron density around HEM C 602:

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

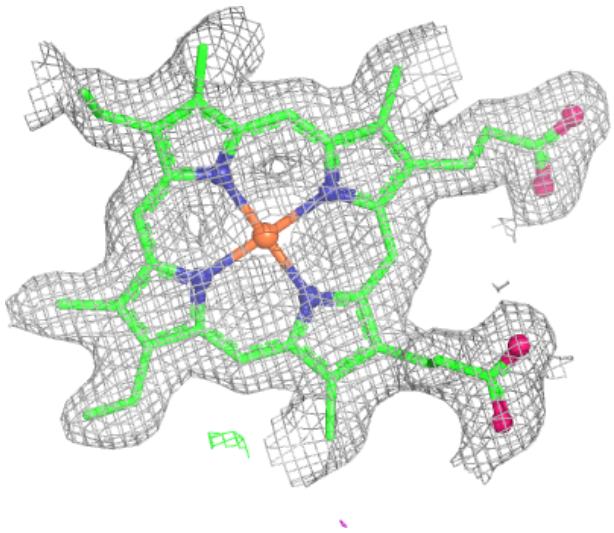


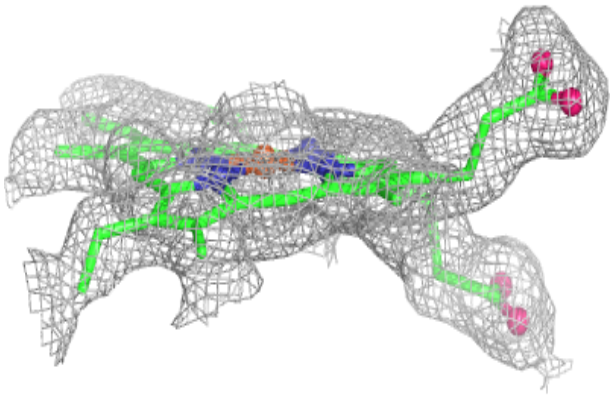


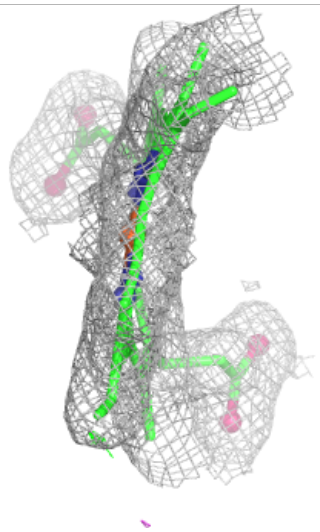


Electron density around HEM D 601:

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

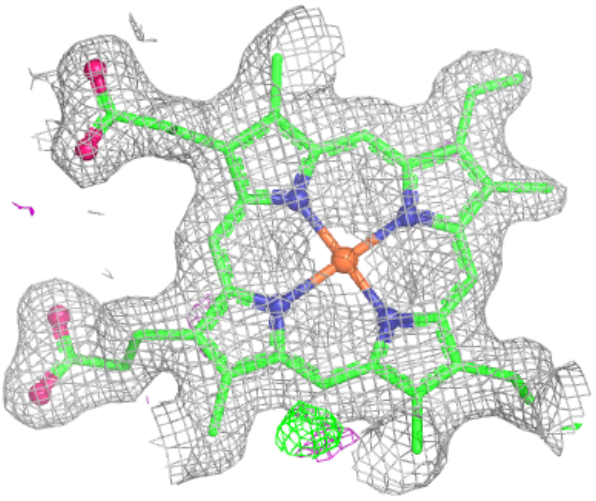


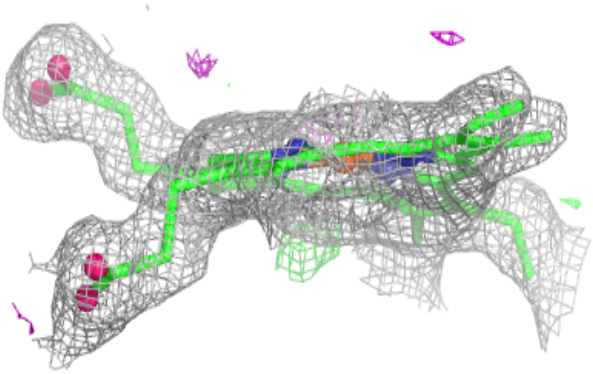


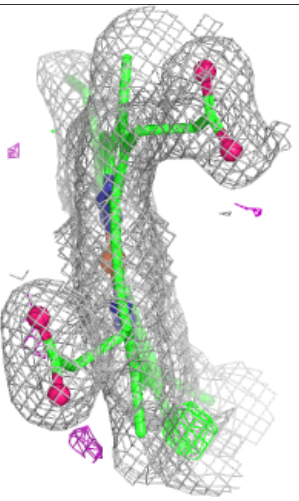


Electron density around HEM G 601:

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

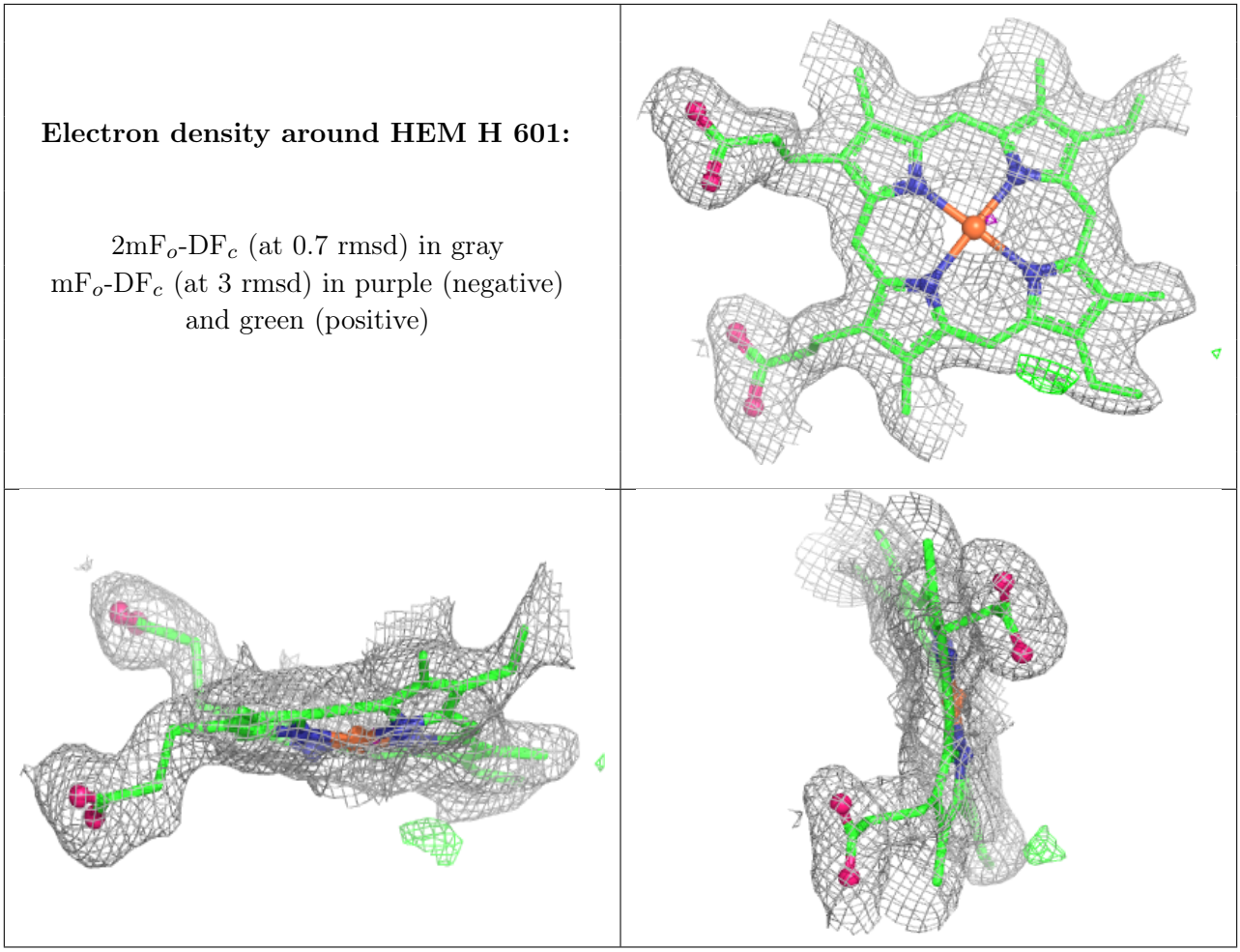






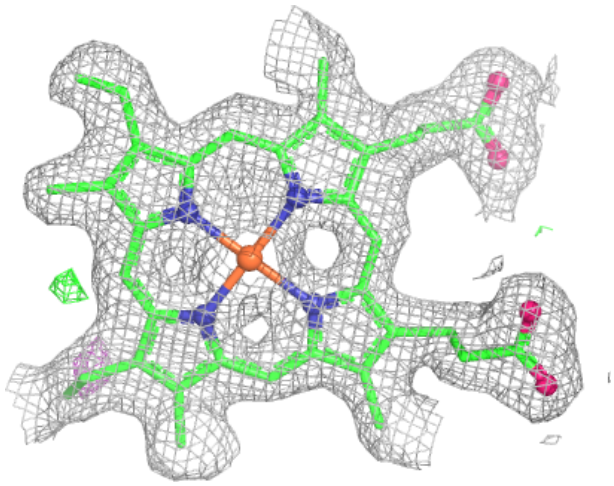
Electron density around HEM H 601:

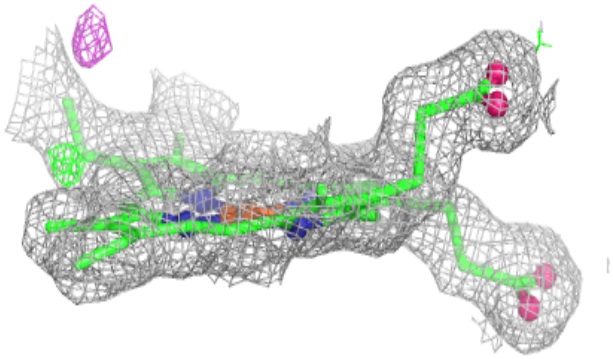
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

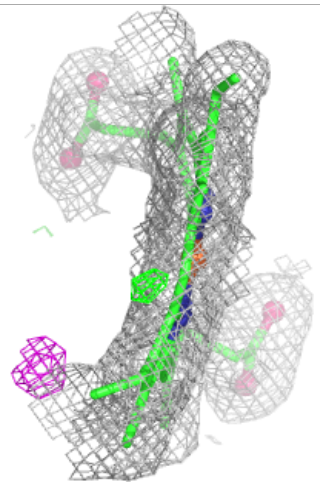


Electron density around HEM K 601:

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

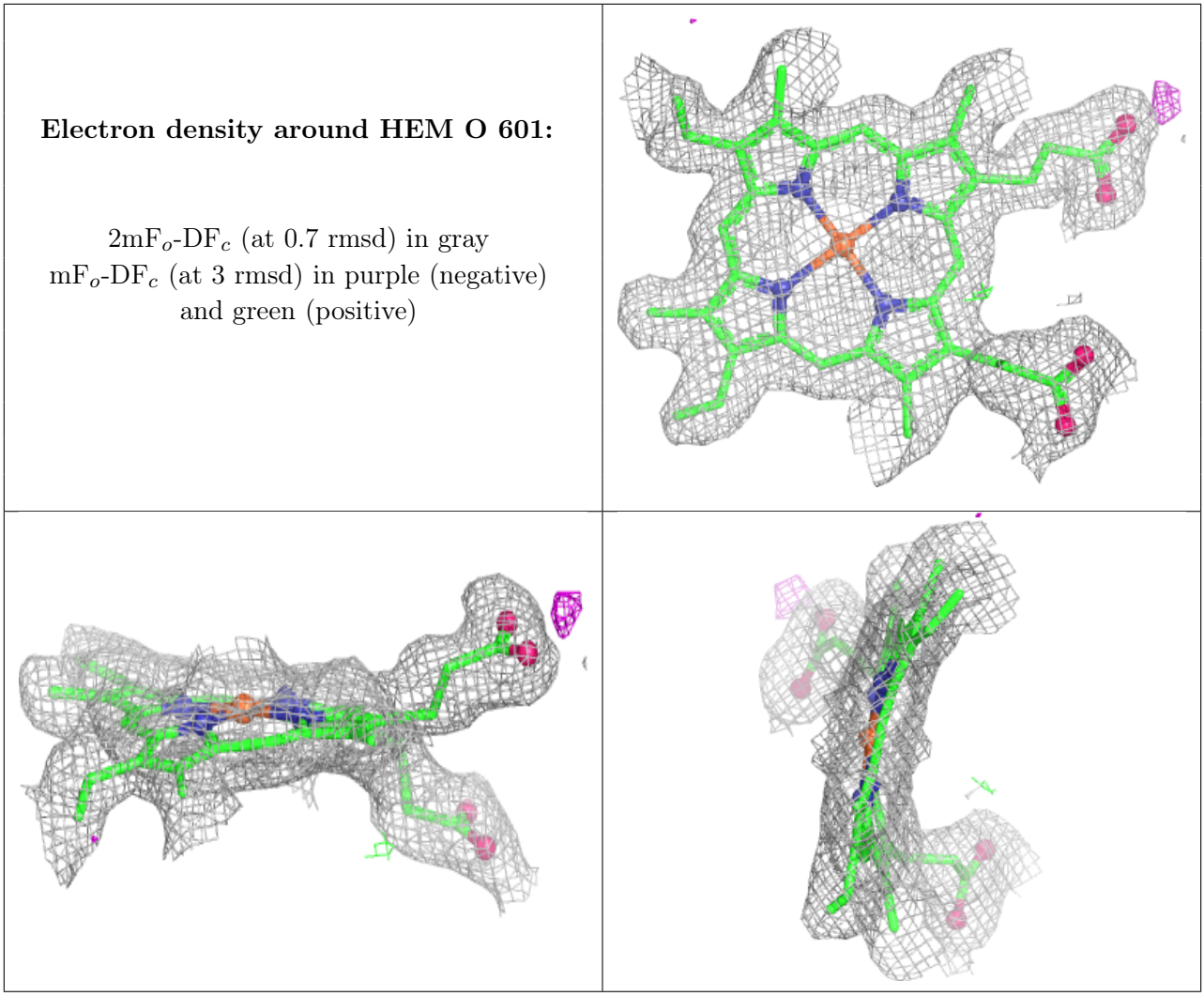






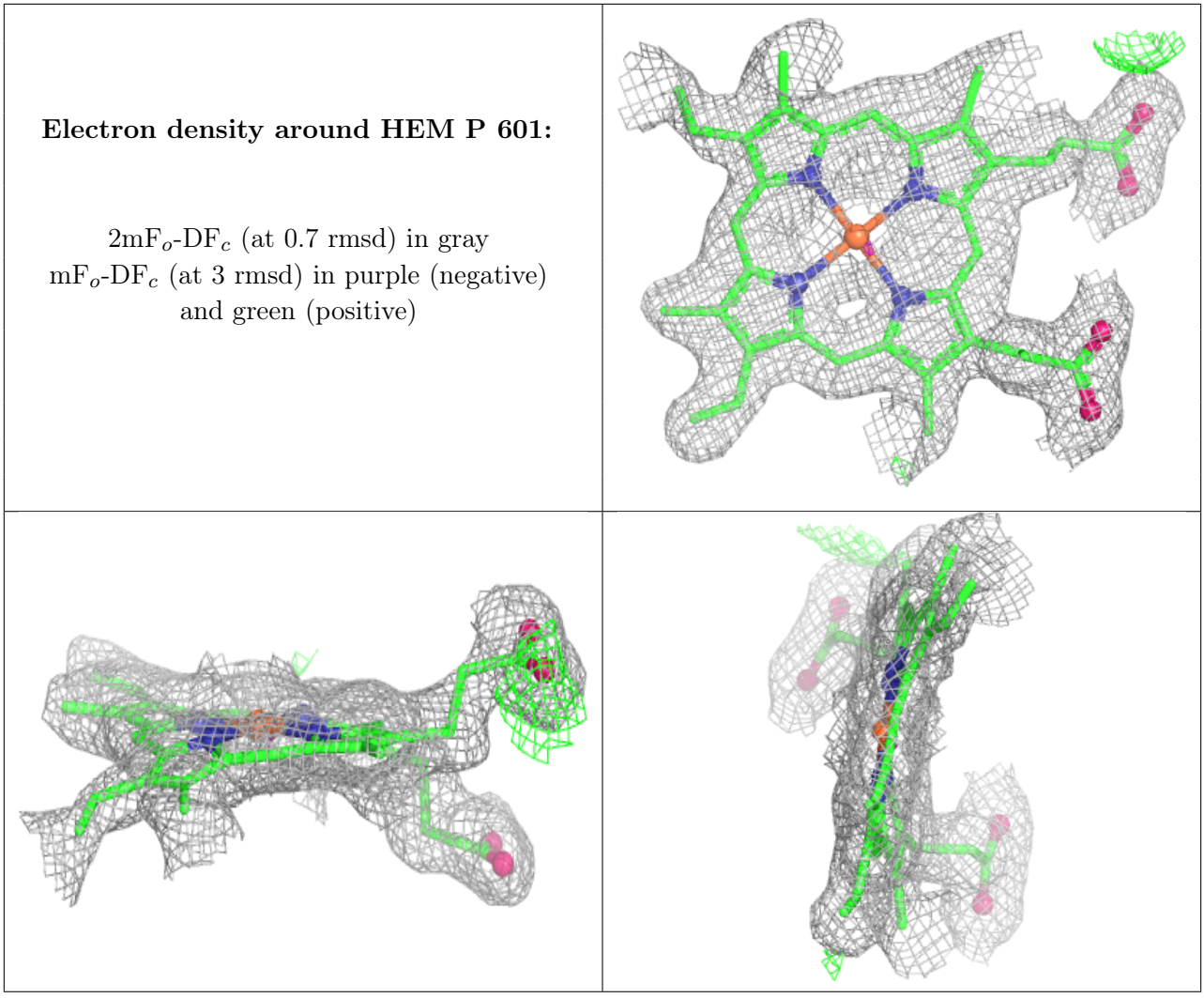
Electron density around HEM O 601:

$2mF_o$-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 P 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.