



wwPDB X-ray Structure Validation Summary Report ⓘ

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-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

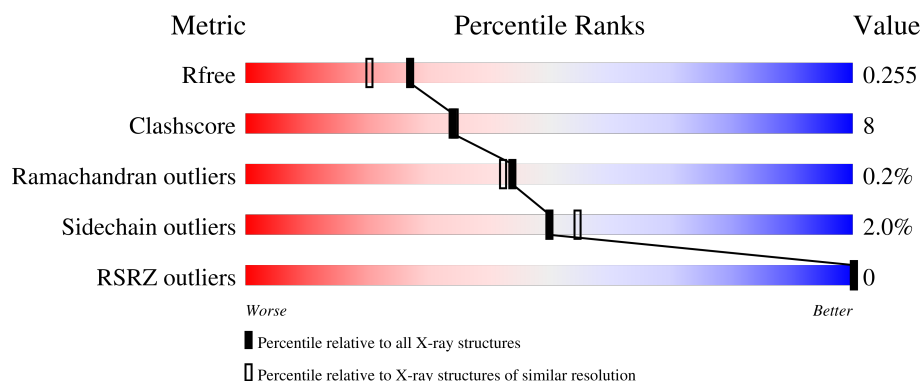
1 Overall quality at a glance

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.



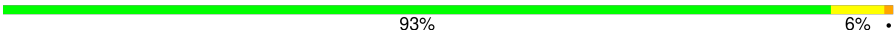









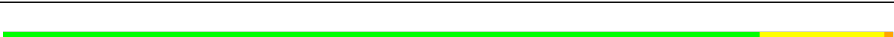
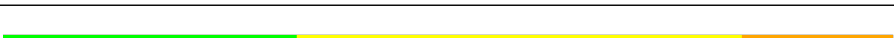

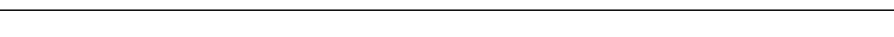
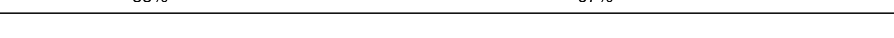
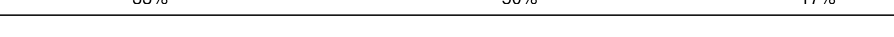

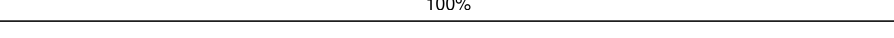

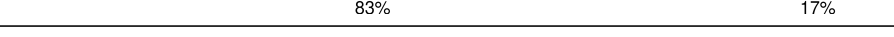
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	104	 91% 9%
1	B	104	 83% 17%
1	E	104	 81% 19%
1	F	104	 78% 21% •
1	I	104	 83% 15% •

Continued on next page...

Continued from previous page...

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.

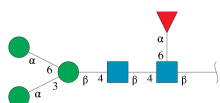
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	465	Total	C	N	O	S	0	1	0
			3726	2348	686	665	27			
2	D	466	Total	C	N	O	S	0	0	0
			3729	2349	687	666	27			
2	G	465	Total	C	N	O	S	0	0	0
			3727	2348	686	666	27			
2	H	466	Total	C	N	O	S	0	0	0
			3729	2349	687	666	27			
2	K	465	Total	C	N	O	S	0	0	0
	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

Continued on next page...

Continued from previous page...

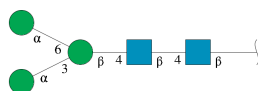
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	466	Total	C	N	O	S	0	0	0
			3729	2349	687	666	27			
2	P	466	Total	C	N	O	S	0	0	0
			3733	2351	687	668	27			

- 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.

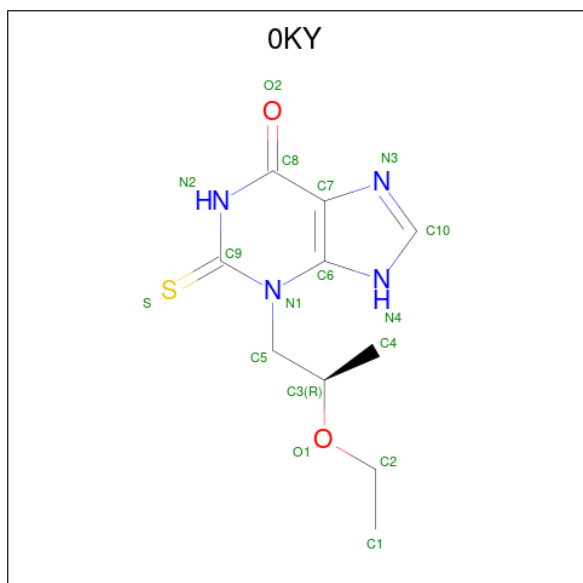


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Y	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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: OKY) (formula: C₁₀H₁₄N₄O₂S).



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

Continued on next page...

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

- # HEM
-
- The diagram illustrates the chemical structure of Hemoglobin (HEM). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The iron atom is also coordinated by a proximal histidine residue (NA) and a distal water molecule (OH). The structure includes various side chains labeled with green text, such as CAA, CBA, CAD, CBD, CMA, C3A, C2A, C4A, C3B, C4B, C1B, C2B, CMB, C3C, C4C, C1C, C2C, CMC, C3D, C4D, C1D, C2D, CMD, C5D, C6D, C7D, C8D, C9D, C10D, C11D, C12D, C13D, C14D, C15D, C16D, C17D, C18D, C19D, C20D, C21D, C22D, C23D, C24D, C25D, C26D, C27D, C28D, C29D, C30D, C31D, C32D, C33D, C34D, C35D, C36D, C37D, C38D, C39D, C40D, C41D, C42D, C43D, C44D, C45D, C46D, C47D, C48D, C49D, C50D, C51D, C52D, C53D, C54D, C55D, C56D, C57D, C58D, C59D, C60D, C61D, C62D, C63D, C64D, C65D, C66D, C67D, C68D, C69D, C70D, C71D, C72D, C73D, C74D, C75D, C76D, C77D, C78D, C79D, C80D, C81D, C82D, C83D, C84D, C85D, C86D, C87D, C88D, C89D, C90D, C91D, C92D, C93D, C94D, C95D, C96D, C97D, C98D, C99D, C100D, C101D, C102D, C103D, C104D, C105D, C106D, C107D, C108D, C109D, C110D, C111D, C112D, C113D, C114D, C115D, C116D, C117D, C118D, C119D, C120D, C121D, C122D, C123D, C124D, C125D, C126D, C127D, C128D, C129D, C130D, C131D, C132D, C133D, C134D, C135D, C136D, C137D, C138D, C139D, C140D, C141D, C142D, C143D, C144D, C145D, C146D, C147D, C148D, C149D, C150D, C151D, C152D, C153D, C154D, C155D, C156D, C157D, C158D, C159D, C160D, C161D, C162D, C163D, C164D, C165D, C166D, C167D, C168D, C169D, C170D, C171D, C172D, C173D, C174D, C175D, C176D, C177D, C178D, C179D, C180D, C181D, C182D, C183D, C184D, C185D, C186D, C187D, C188D, C189D, C190D, C191D, C192D, C193D, C194D, C195D, C196D, C197D, C198D, C199D, C200D, C201D, C202D, C203D, C204D, C205D, C206D, C207D, C208D, C209D, C210D, C211D, C212D, C213D, C214D, C215D, C216D, C217D, C218D, C219D, C220D, C221D, C222D, C223D, C224D, C225D, C226D, C227D, C228D, C229D, C230D, C231D, C232D, C233D, C234D, C235D, C236D, C237D, C238D, C239D, C240D, C241D, C242D, C243D, C244D, C245D, C246D, C247D, C248D, C249D, C250D, C251D, C252D, C253D, C254D, C255D, C256D, C257D, C258D, C259D, C260D, C261D, C262D, C263D, C264D, C265D, C266D, C267D, C268D, C269D, C270D, C271D, C272D, C273D, C274D, C275D, C276D, C277D, C278D, C279D, C280D, C281D, C282D, C283D, C284D, C285D, C286D, C287D, C288D, C289D, C290D, C291D, C292D, C293D, C294D, C295D, C296D, C297D, C298D, C299D, C300D, C301D, C302D, C303D, C304D, C305D, C306D, C307D, C308D, C309D, C310D, C311D, C312D, C313D, C314D, C315D, C316D, C317D, C318D, C319D, C320D, C321D, C322D, C323D, C324D, C325D, C326D, C327D, C328D, C329D, C330D, C331D, C332D, C333D, C334D, C335D, C336D, C337D, C338D, C339D, C340D, C341D, C342D, C343D, C344D, C345D, C346D, C347D, C348D, C349D, C350D, C351D, C352D, C353D, C354D, C355D, C356D, C357D, C358D, C359D, C360D, C361D, C362D, C363D, C364D, C365D, C366D, C367D, C368D, C369D, C370D, C371D, C372D, C373D, C374D, C375D, C376D, C377D, C378D, C379D, C380D, C381D, C382D, C383D, C384D, C385D, C386D, C387D, C388D, C389D, C390D, C391D, C392D, C393D, C394D, C395D, C396D, C397D, C398D, C399D, C400D, C401D, C402D, C403D, C404D, C405D, C406D, C407D, C408D, C409D, C410D, C411D, C412D, C413D, C414D, C415D, C416D, C417D, C418D, C419D, C420D, C421D, C422D, C423D, C424D, C425D, C426D, C427D, C428D, C429D, C430D, C431D, C432D, C433D, C434D, C435D, C436D, C437D, C438D, C439D, C440D, C441D, C442D, C443D, C444D, C445D, C446D, C447D, C448D, C449D, C450D, C451D, C452D, C453D, C454D, C455D, C456D, C457D, C458D, C459D, C460D, C461D, C462D, C463D, C464D, C465D, C466D, C467D, C468D, C469D, C470D, C471D, C472D, C473D, C474D, C475D, C476D, C477D, C478D, C479D, C480D, C481D, C482D, C483D, C484D, C485D, C486D, C487D, C488D, C489D, C490D, C491D, C492D, C493D, C494D, C495D, C496D, C497D, C498D, C499D, C500D, C501D, C502D, C503D, C504D, C505D, C506D, C507D, C508D, C509D, C510D, C511D, C512D, C513D, C514D, C515D, C516D, C517D, C518D, C519D, C520D, C521D, C522D, C523D, C524D, C525D, C526D, C527D, C528D, C529D, C530D, C531D, C532D, C533D, C534D, C535D, C536D, C537D, C538D, C539D, C540D, C541D, C542D, C543D, C544D, C545D, C546D, C547D, C548D, C549D, C550D, C551D, C552D, C553D, C554D, C555D, C556D, C557D, C558D, C559D, C560D, C561D, C562D, C563D, C564D, C565D, C566D, C567D, C568D, C569D, C570D, C571D, C572D, C573D, C574D, C575D, C576D, C577D, C578D, C579D, C580D, C581D, C582D, C583D, C584D, C585D, C586D, C587D, C588D, C589D, C590D, C591D, C592D, C593D, C594D, C595D, C596D, C597D, C598D, C599D, C600D, C601D, C602D, C603D, C604D, C605D, C606D, C607D, C608D, C609D, C610D, C611D, C612D, C613D, C614D, C615D, C616D, C617D, C618D, C619D, C620D, C621D, C622D, C623D, C624D, C625D, C626D, C627D, C628D, C629D, C630D, C631D, C632D, C633D, C634D, C635D, C636D, C637D, C638D, C639D, C640D, C641D, C642D, C643D, C644D, C645D, C646D, C647D, C648D, C649D, C650D, C651D, C652D, C653D, C654D, C655D, C656D, C657D, C658D, C659D, C660D, C661D, C662D, C663D, C664D, C665D, C666D, C667D, C66

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



WORLD WIDE
PDB
PROTEIN DATA BANK

Continued from previous page...

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

- 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		

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 10 is water.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	74	Total 74	O 74	0	0
10	D	271	Total 271	O 271	0	0
10	E	64	Total 64	O 64	0	0
10	G	243	Total 243	O 243	0	0
10	F	73	Total 73	O 73	0	0
10	H	199	Total 199	O 199	0	0
10	I	72	Total 72	O 72	0	0
10	K	214	Total 214	O 214	0	0
10	J	66	Total 66	O 66	0	0
10	L	252	Total 252	O 252	0	0
10	M	67	Total 67	O 67	0	0
10	O	227	Total 227	O 227	0	0
10	N	62	Total 62	O 62	0	0
10	P	215	Total 215	O 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:  91% 9%




- Molecule 1: Myeloperoxidase light chain

Chain B:  83% 17%



- Molecule 1: Myeloperoxidase light chain

Chain E:  81% 19%




- Molecule 1: Myeloperoxidase light chain

Chain F:  78% 21%



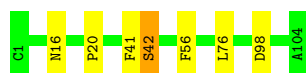
- Molecule 1: Myeloperoxidase light chain

Chain I:  83% 15%



- Molecule 1: Myeloperoxidase light chain

Chain J:  93% 6%



- Molecule 1: Myeloperoxidase light chain

Chain M: 85% 14%



- Molecule 1: Myeloperoxidase light chain

Chain N: 85% 15%



- Molecule 2: Myeloperoxidase heavy chain

Chain C: 86% 13%



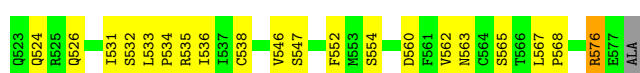
- Molecule 2: Myeloperoxidase heavy chain

Chain D: 86% 13%

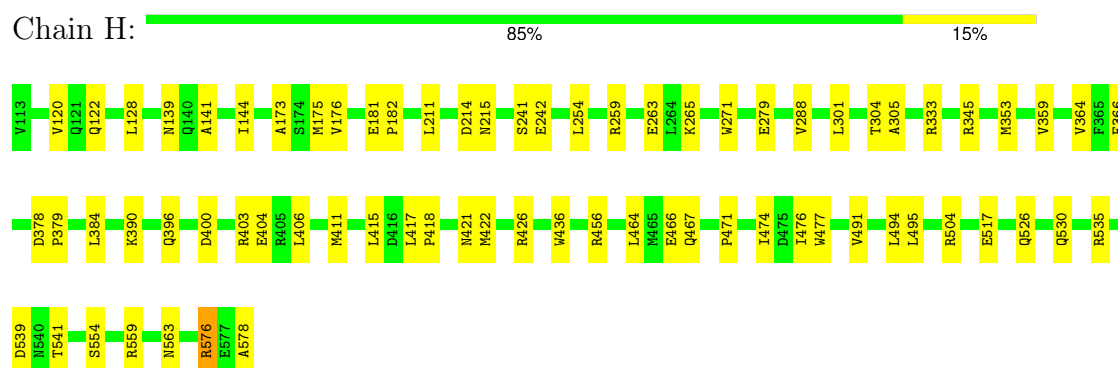


- Molecule 2: Myeloperoxidase heavy chain

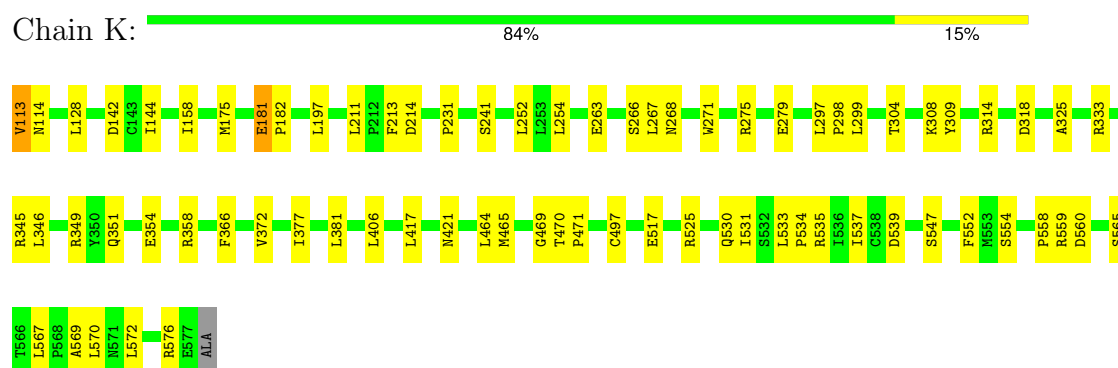
Chain G: 80% 18%



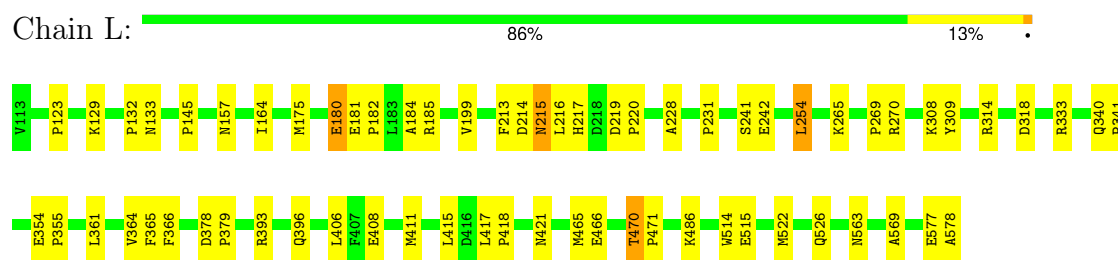
• Molecule 2: Myeloperoxidase heavy chain



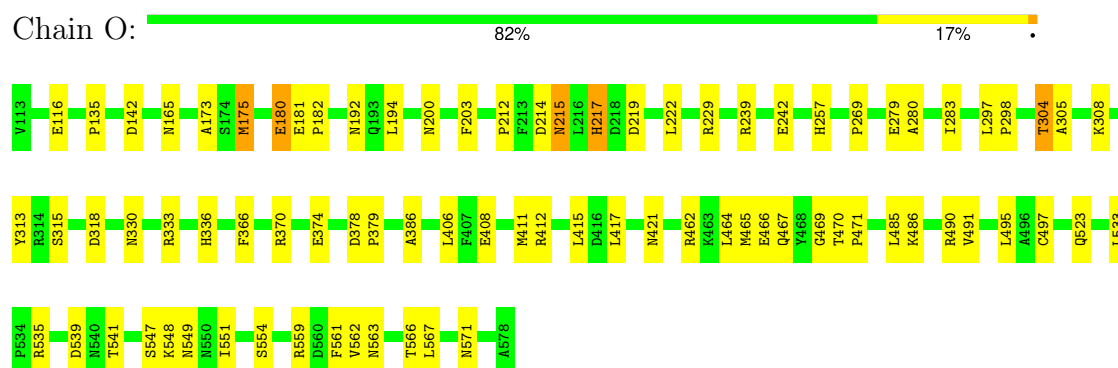
• Molecule 2: Myeloperoxidase heavy chain




• Molecule 2: Myeloperoxidase heavy chain

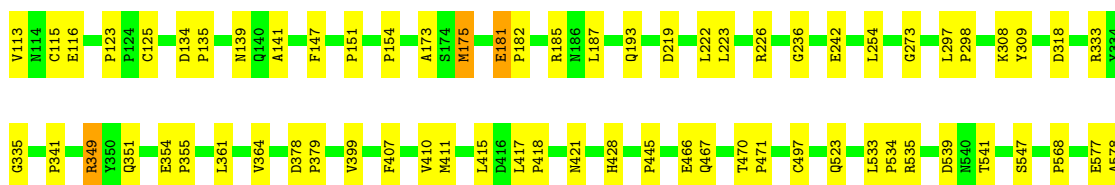


• Molecule 2: Myeloperoxidase heavy chain



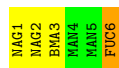
- Molecule 2: Myeloperoxidase heavy chain

Chain P:  85% 14%

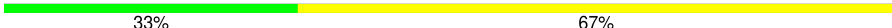


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamid o-2-deoxy-beta-D-glucopyranose

Chain Q:  33% 50% 17%



- 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-acetamid o-2-deoxy-beta-D-glucopyranose

Chain R:  33% 67%



- 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-acetamid o-2-deoxy-beta-D-glucopyranose

Chain S:  33% 67%



- 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-acetamid o-2-deoxy-beta-D-glucopyranose

Chain T:  33% 50% 17%



- 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-acetamid o-2-deoxy-beta-D-glucopyranose

Chain U:  50% 50%

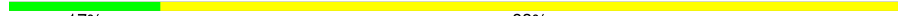


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%




- 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:  17% 83%



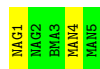
- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  83% 17%



- 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:  60% 40%



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, CSO, MAN, BMA, OKY, 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($^{\circ}$)	Ideal($^{\circ}$)
2	L	318	ASP	CB-CG-OD1	5.26	123.03	118.30

There are no chirality outliers.

5 of 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

5.2 Too-close contacts

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

The worst 5 of 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

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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

5 of 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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	470	THR
1	N	75	GLN
1	M	80	GLN
2	O	330	ASN
2	P	254	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	201	GLN
2	O	217	HIS
2	L	215	ASN
1	M	16	ASN
2	O	421	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	1	NAG	C1-O5-C5	3.94	117.47	112.19

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

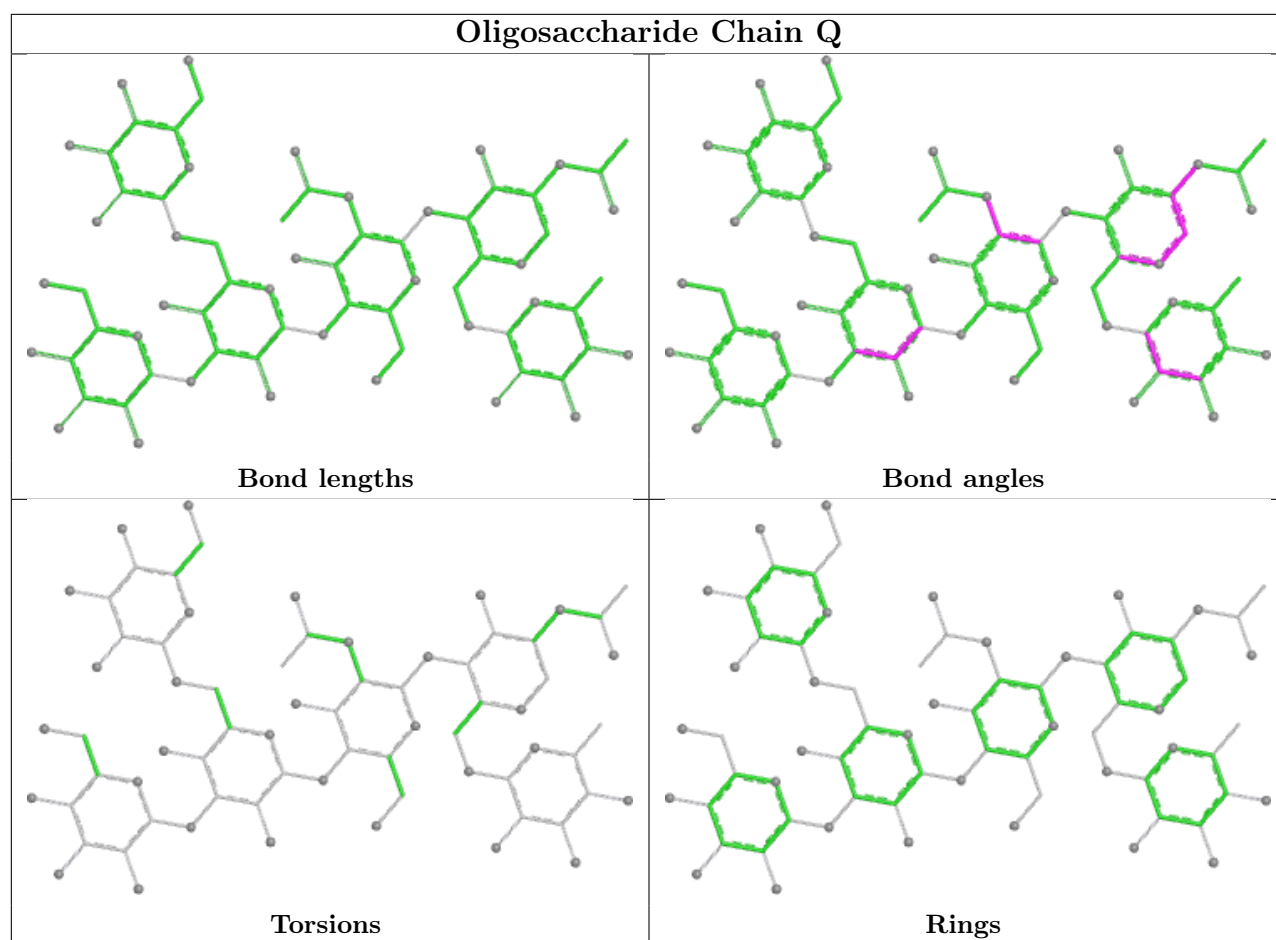
Mol	Chain	Res	Type	Atoms
4	Y	5	MAN	C4-C5-C6-O6
3	S	4	MAN	O5-C5-C6-O6
3	W	4	MAN	O5-C5-C6-O6
4	Y	5	MAN	O5-C5-C6-O6
3	S	4	MAN	C4-C5-C6-O6

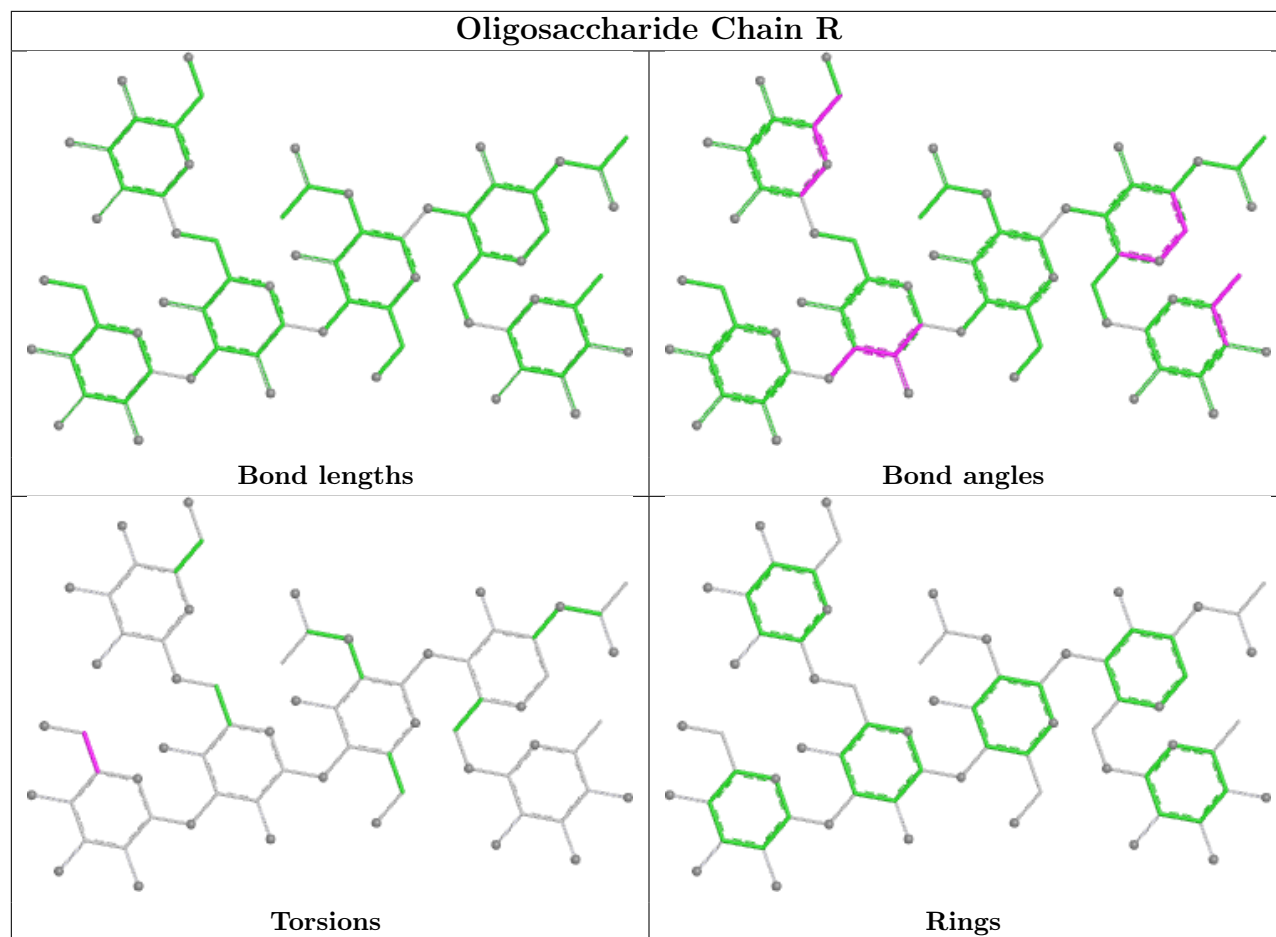
There are no ring outliers.

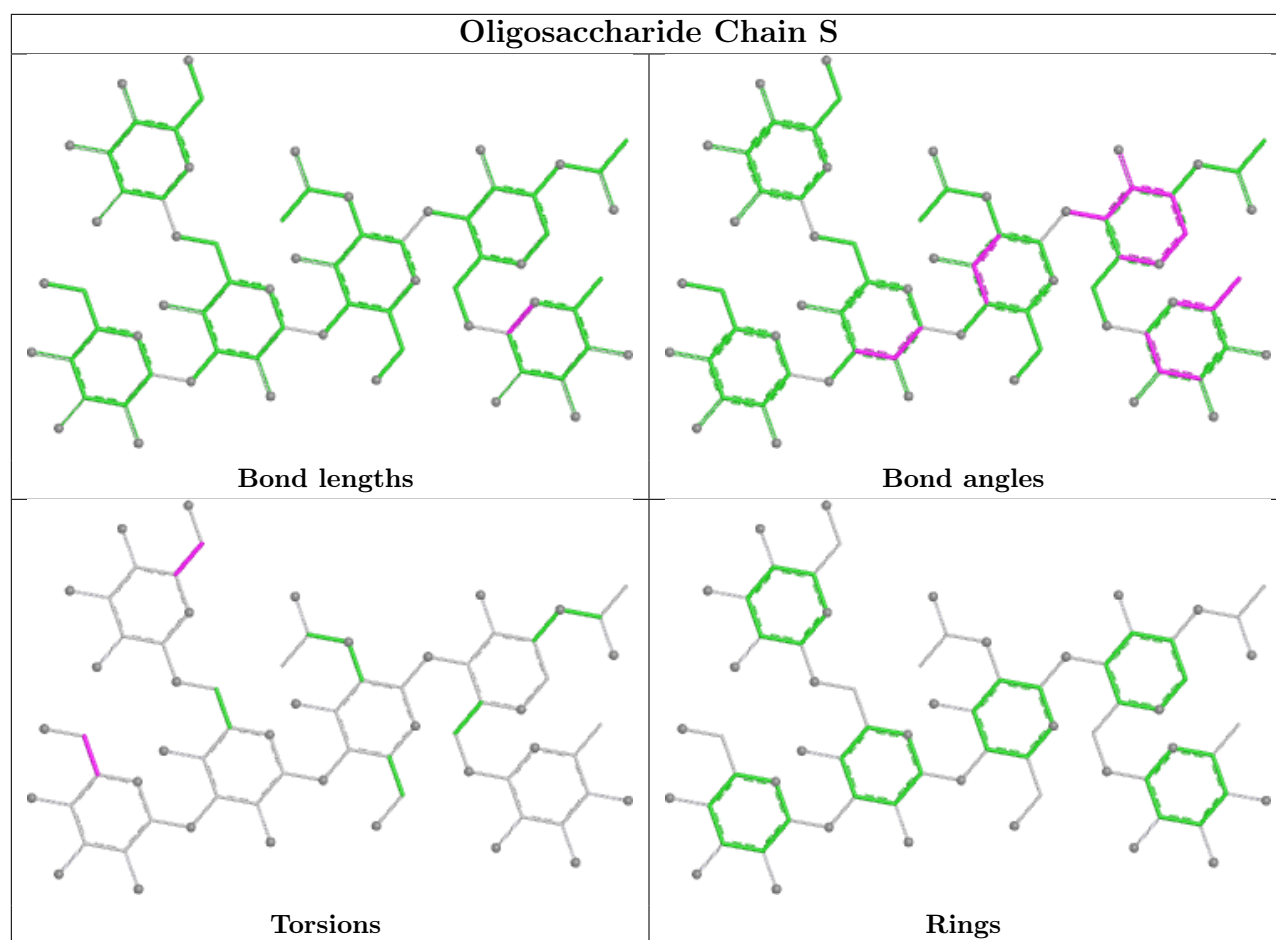
4 monomers are involved in 5 short contacts:

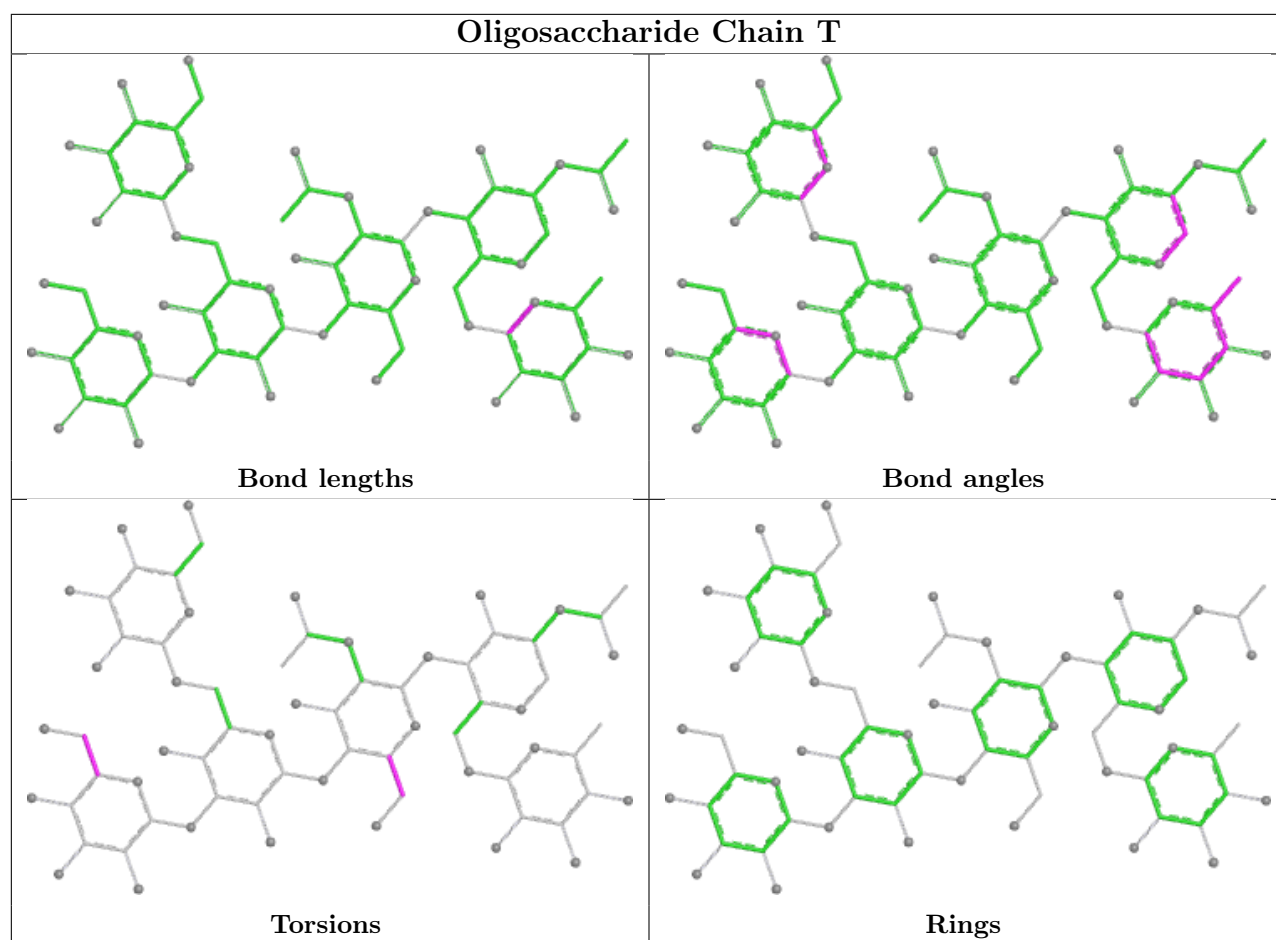
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	W	4	MAN	1	0
3	X	4	MAN	2	0
3	T	4	MAN	1	0
3	Q	6	FUC	1	0

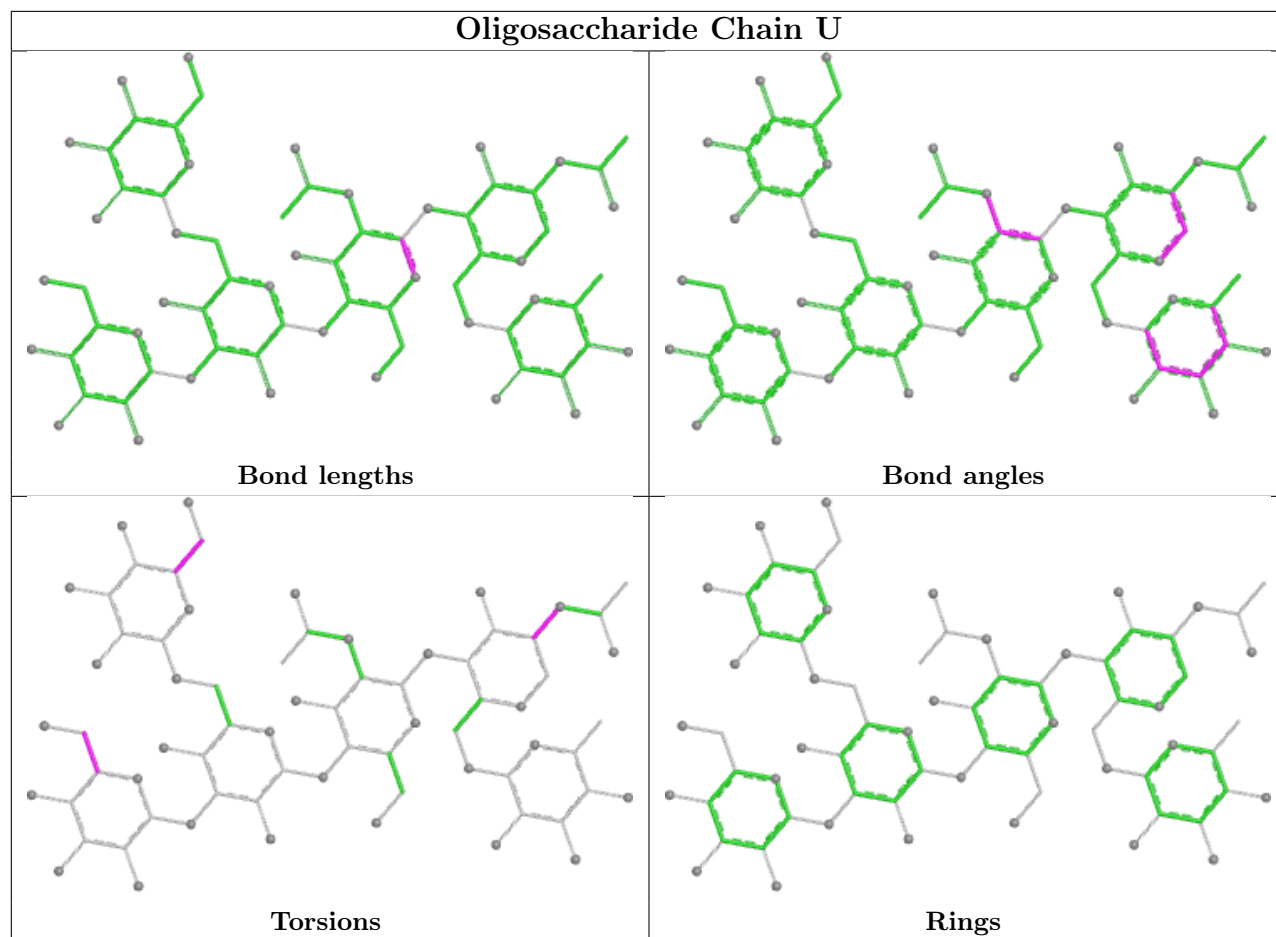
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

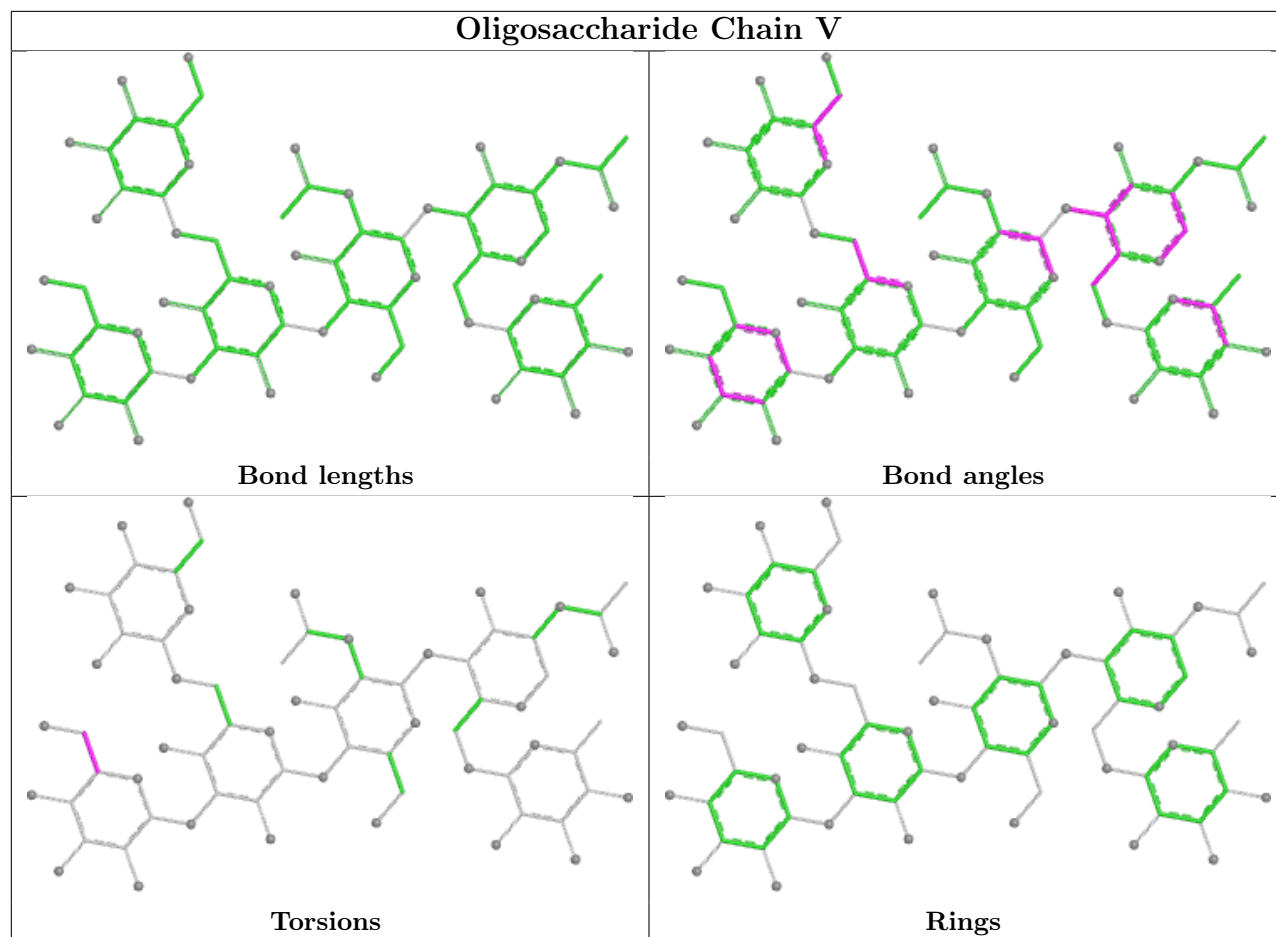


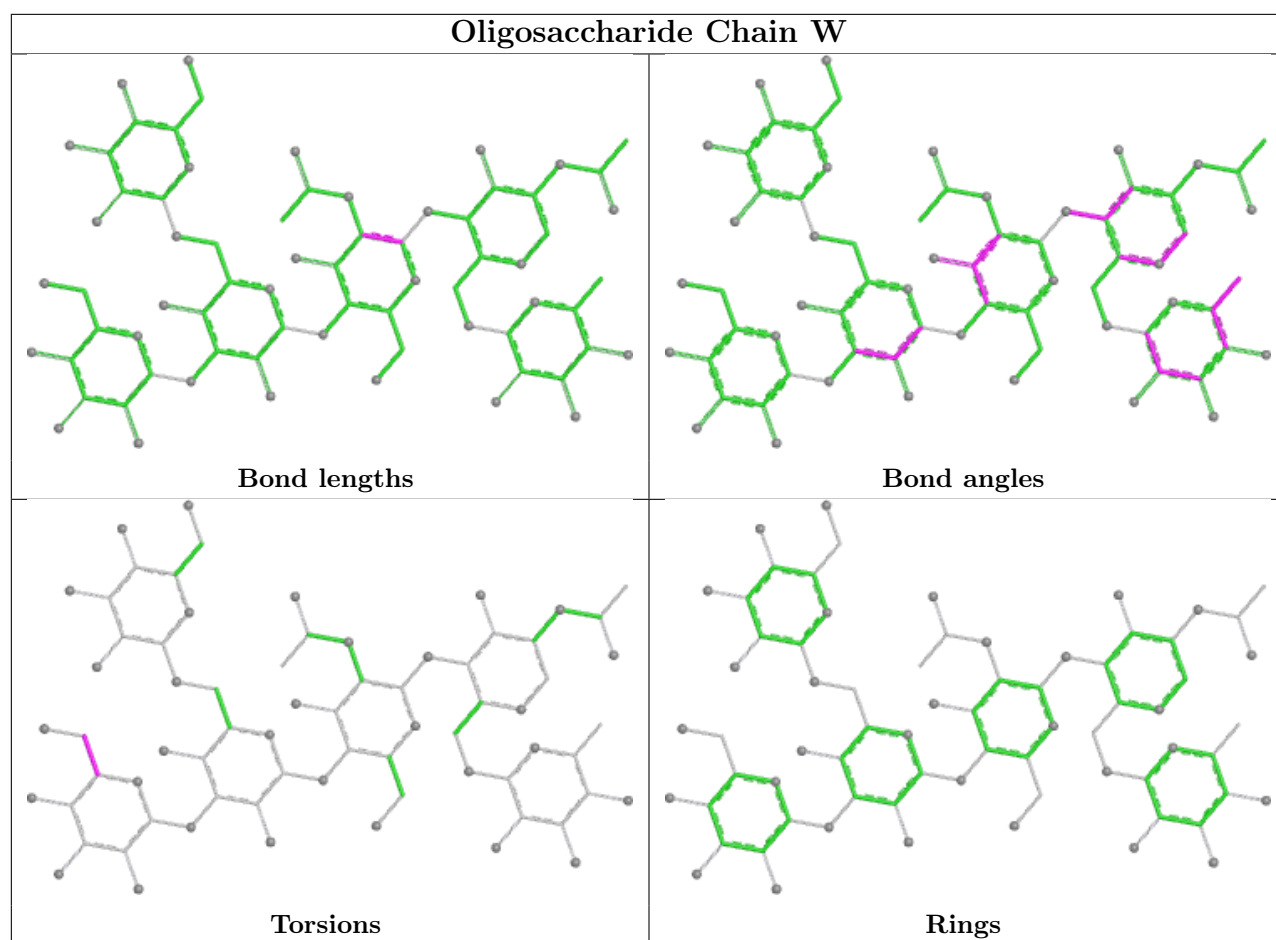


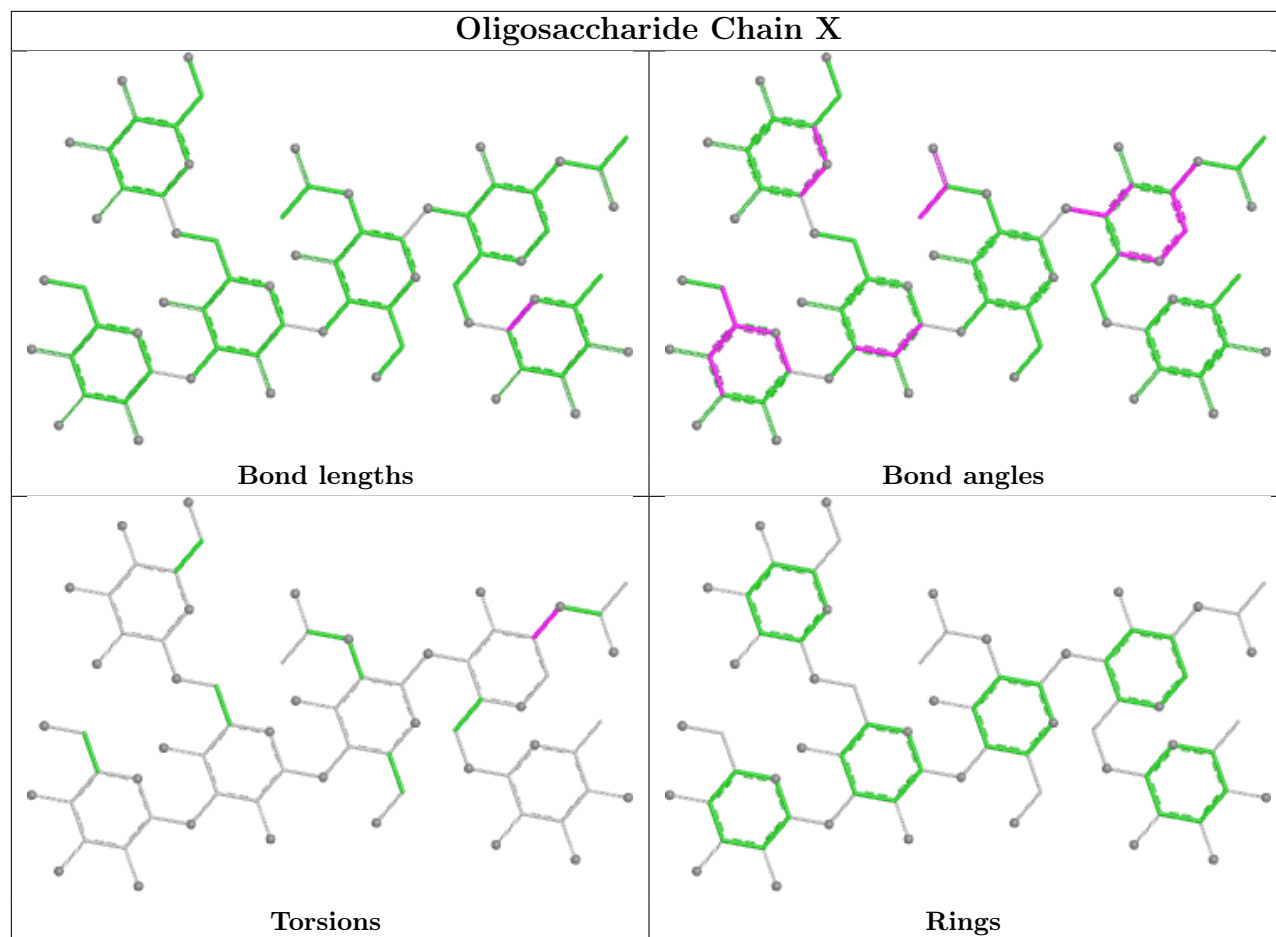


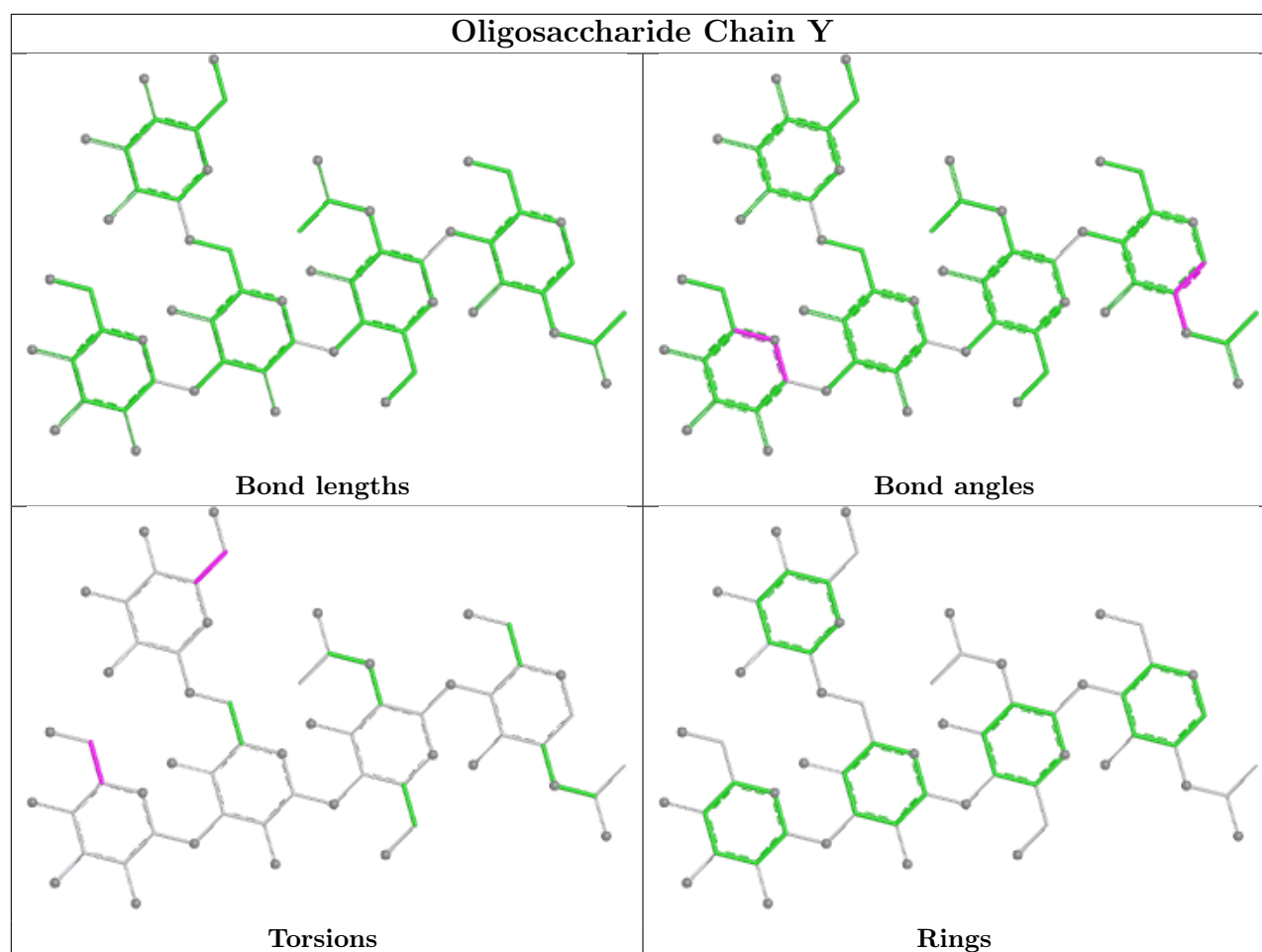












5.6 Ligand geometry [i](#)

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	OKY	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	OKY	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	OKY	C	601	7	14,18,18	2.38	4 (28%)	13,25,25	2.48	4 (30%)
6	OKY	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	OKY	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	OKY	K	602	7	14,18,18	2.26	4 (28%)	13,25,25	2.54	4 (30%)
6	OKY	L	602	7	14,18,18	2.37	4 (28%)	13,25,25	2.29	5 (38%)
6	OKY	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	OKY	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	-

Continued on next page...

Continued from previous page...

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	OKY	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	OKY	C	601	7	-	3/7/7/7	0/2/2/2
6	OKY	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	OKY	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	OKY	K	602	7	-	3/7/7/7	0/2/2/2
6	OKY	L	602	7	-	2/7/7/7	0/2/2/2
6	OKY	H	605	7	-	4/7/7/7	0/2/2/2

The worst 5 of 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

The worst 5 of 122 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 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

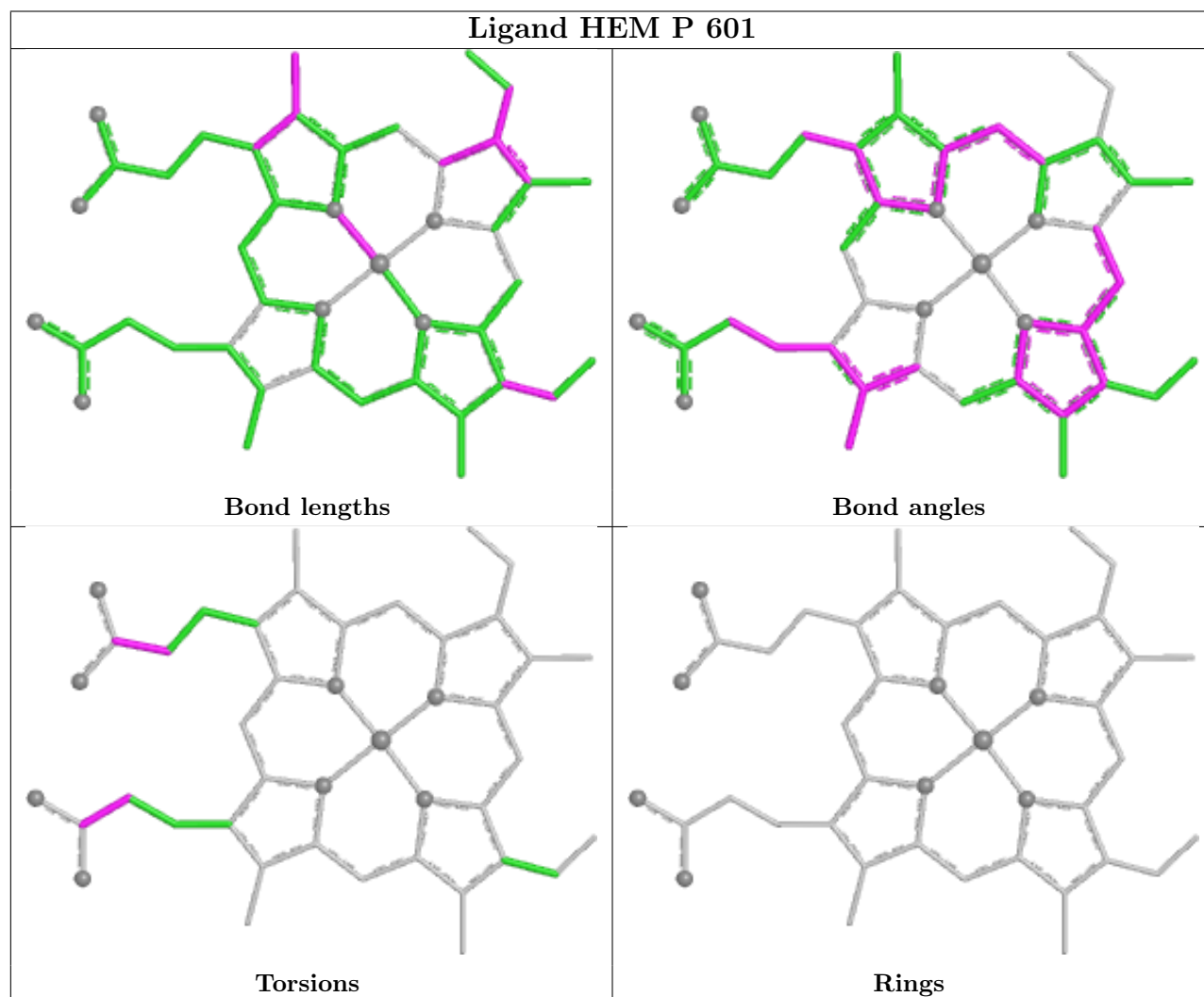
There are no ring outliers.

18 monomers are involved in 57 short contacts:

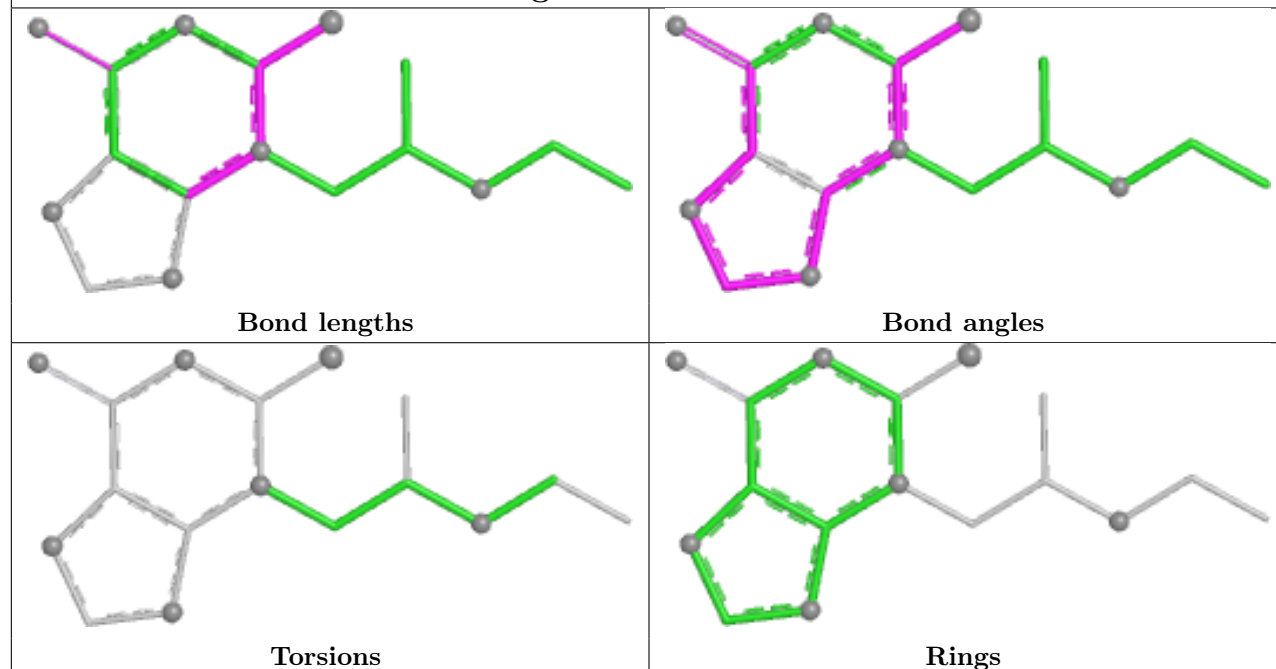
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	601	HEM	7	0
6	G	605	0KY	1	0
8	D	604	NAG	1	0
7	C	602	HEM	6	0
6	D	602	0KY	4	0
7	D	601	HEM	5	0
7	K	601	HEM	1	0
7	L	601	HEM	5	0
7	H	601	HEM	5	0
6	C	601	0KY	3	0
6	O	605	0KY	5	0
7	G	601	HEM	6	0
7	O	601	HEM	5	0
6	P	604	0KY	4	0
8	G	603	NAG	2	0
6	K	602	0KY	2	0
6	L	602	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 than 5% of the Mogul distribution of torsion angles is

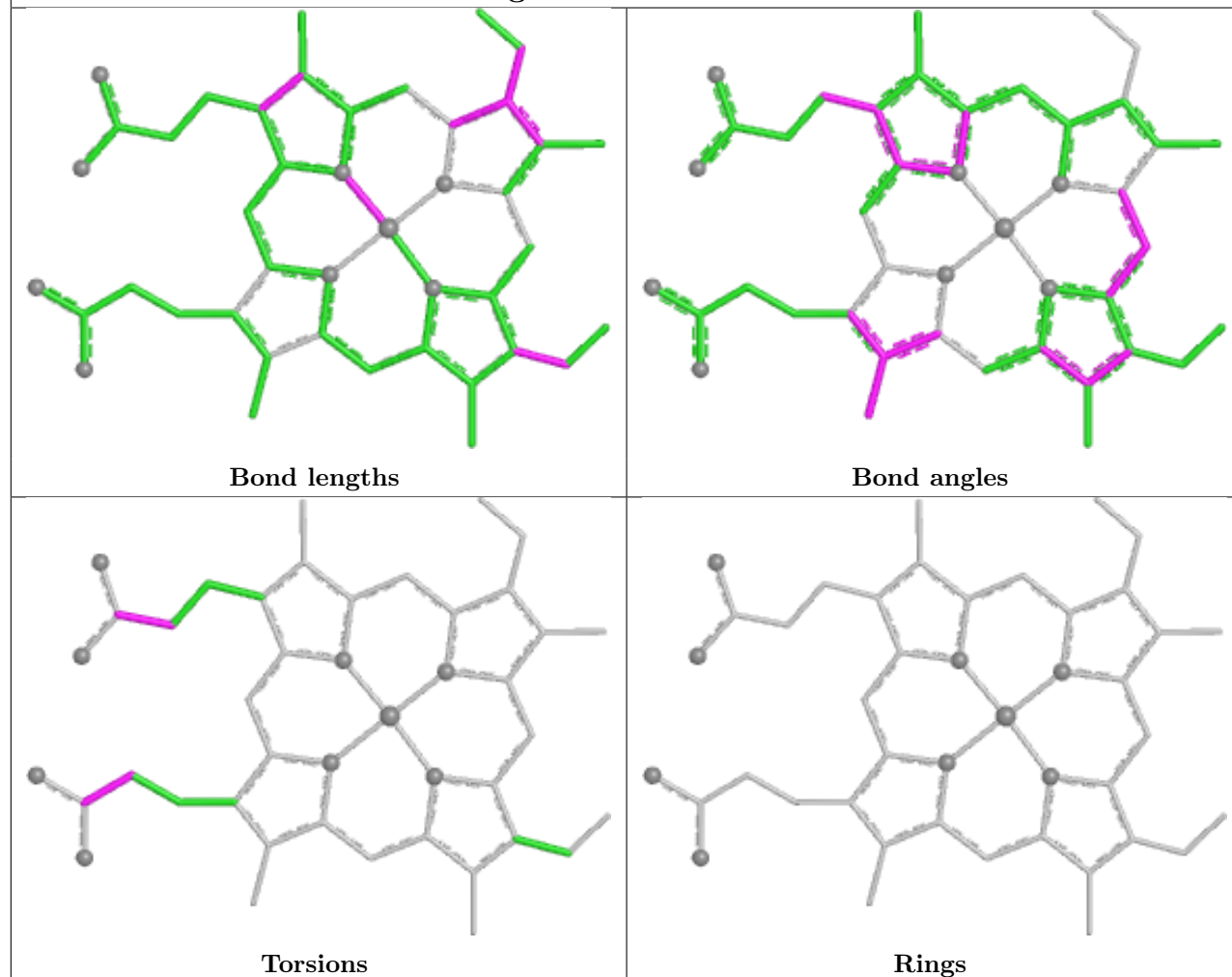
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



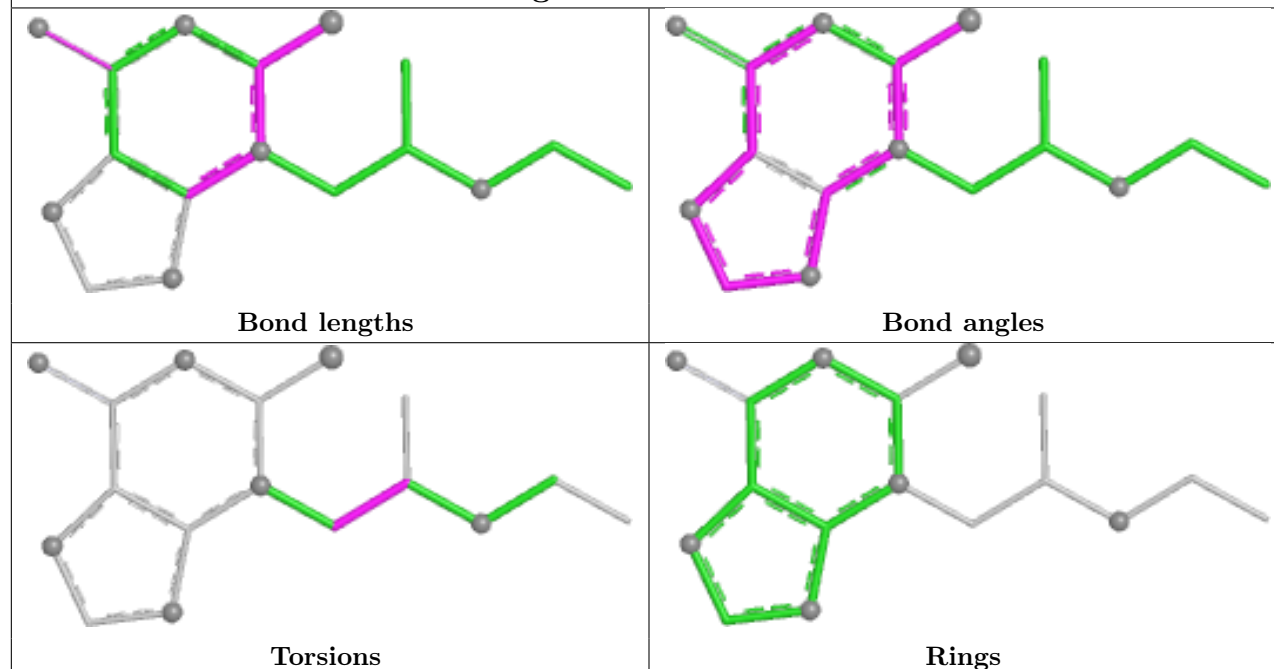
Ligand 0KY G 605



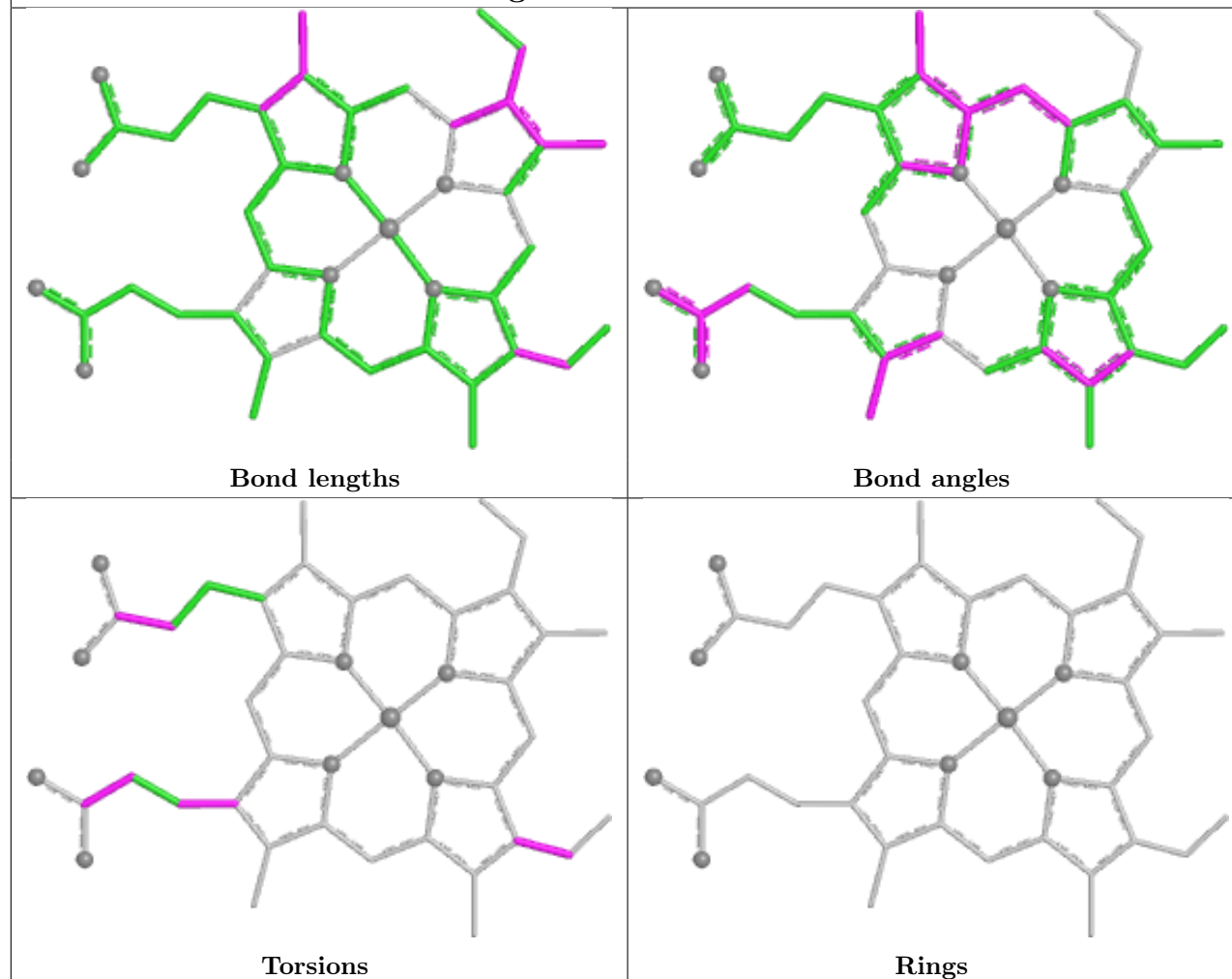
Ligand HEM C 602

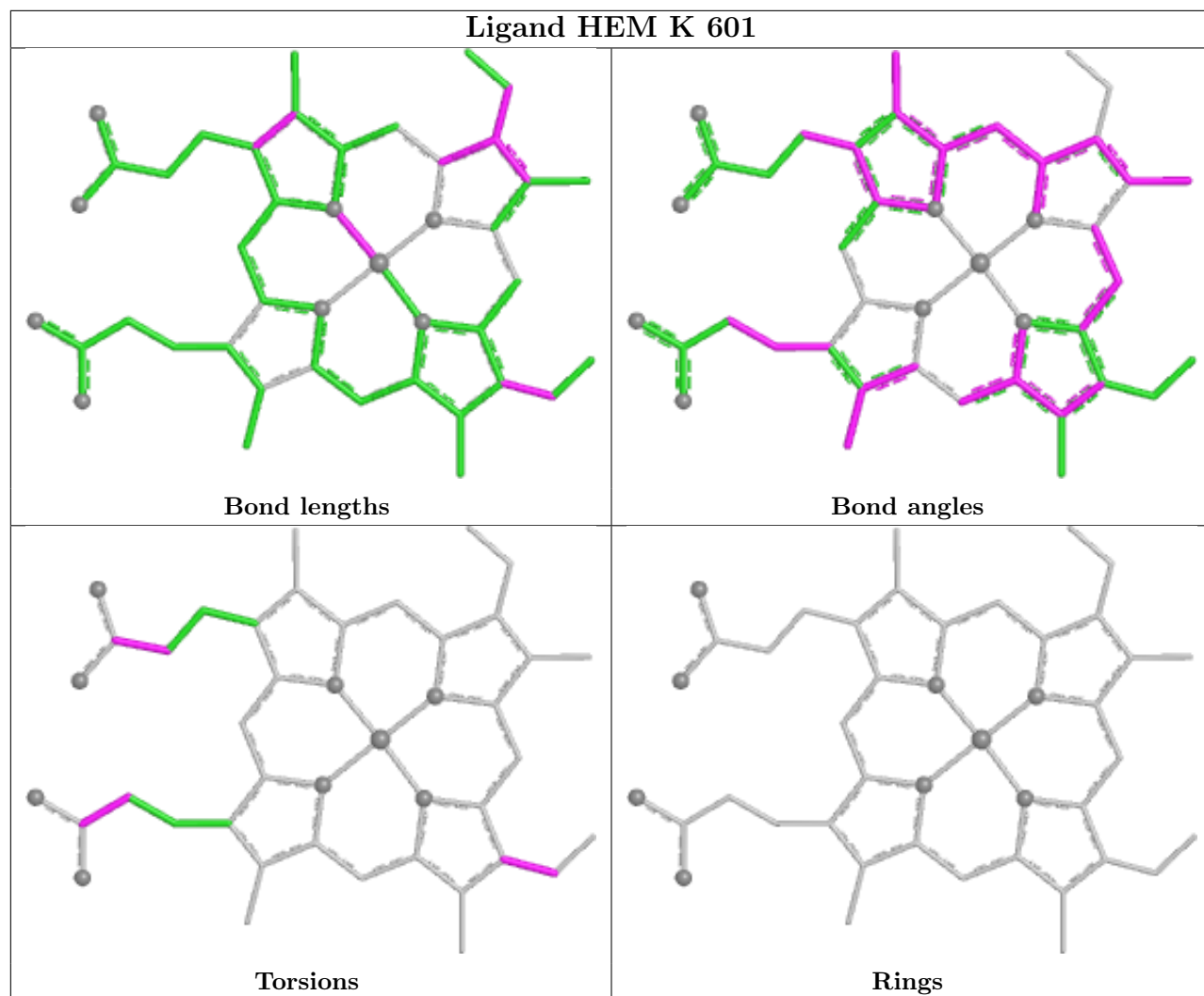


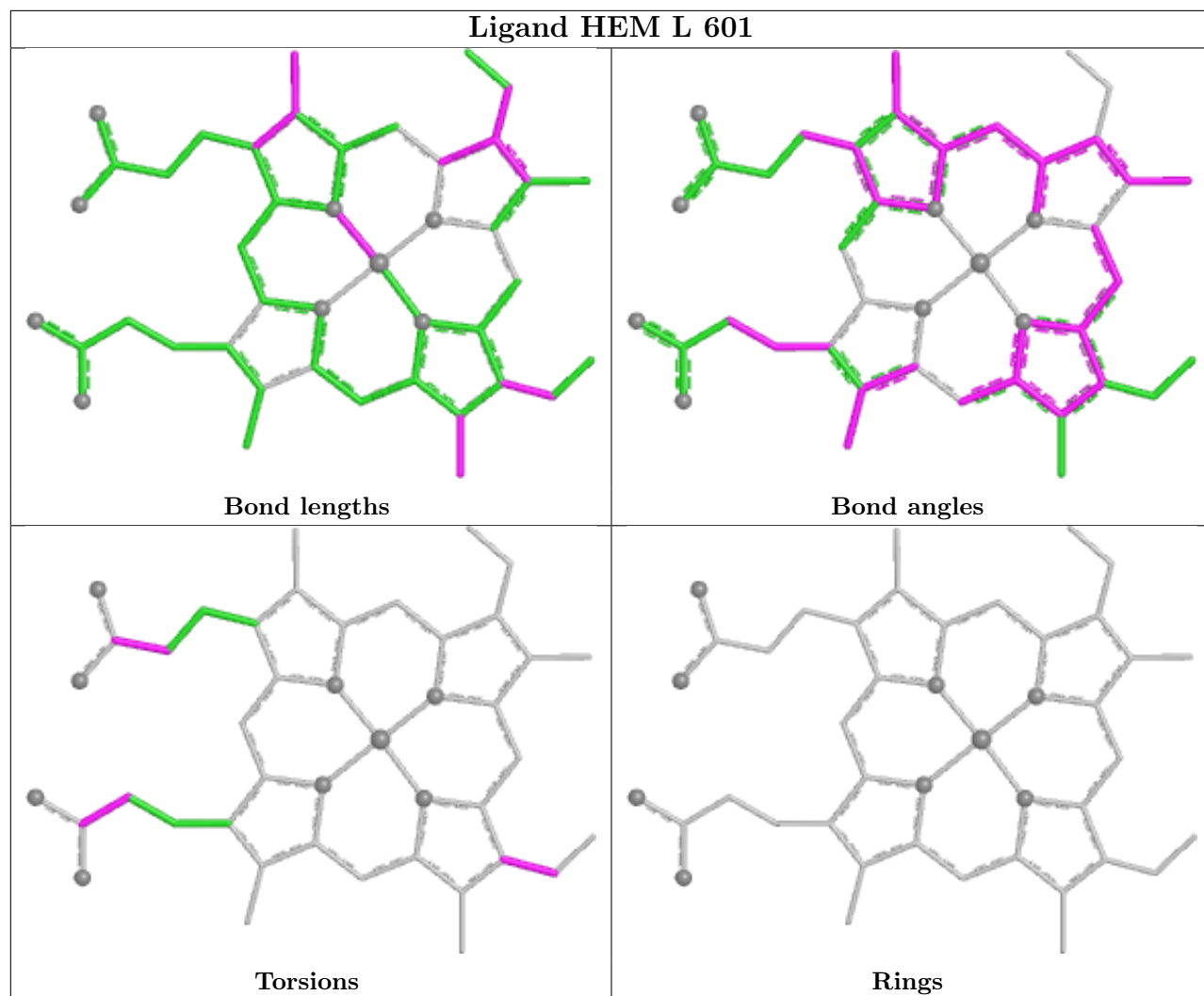
Ligand 0KY D 602

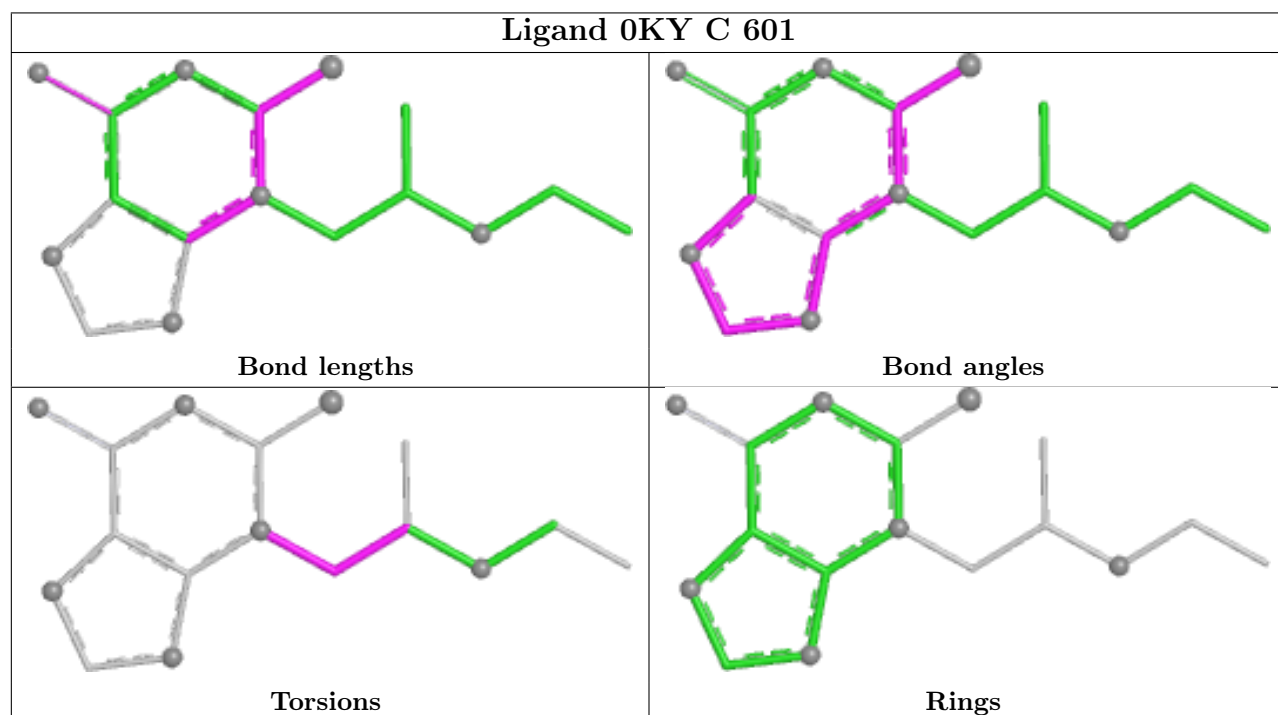
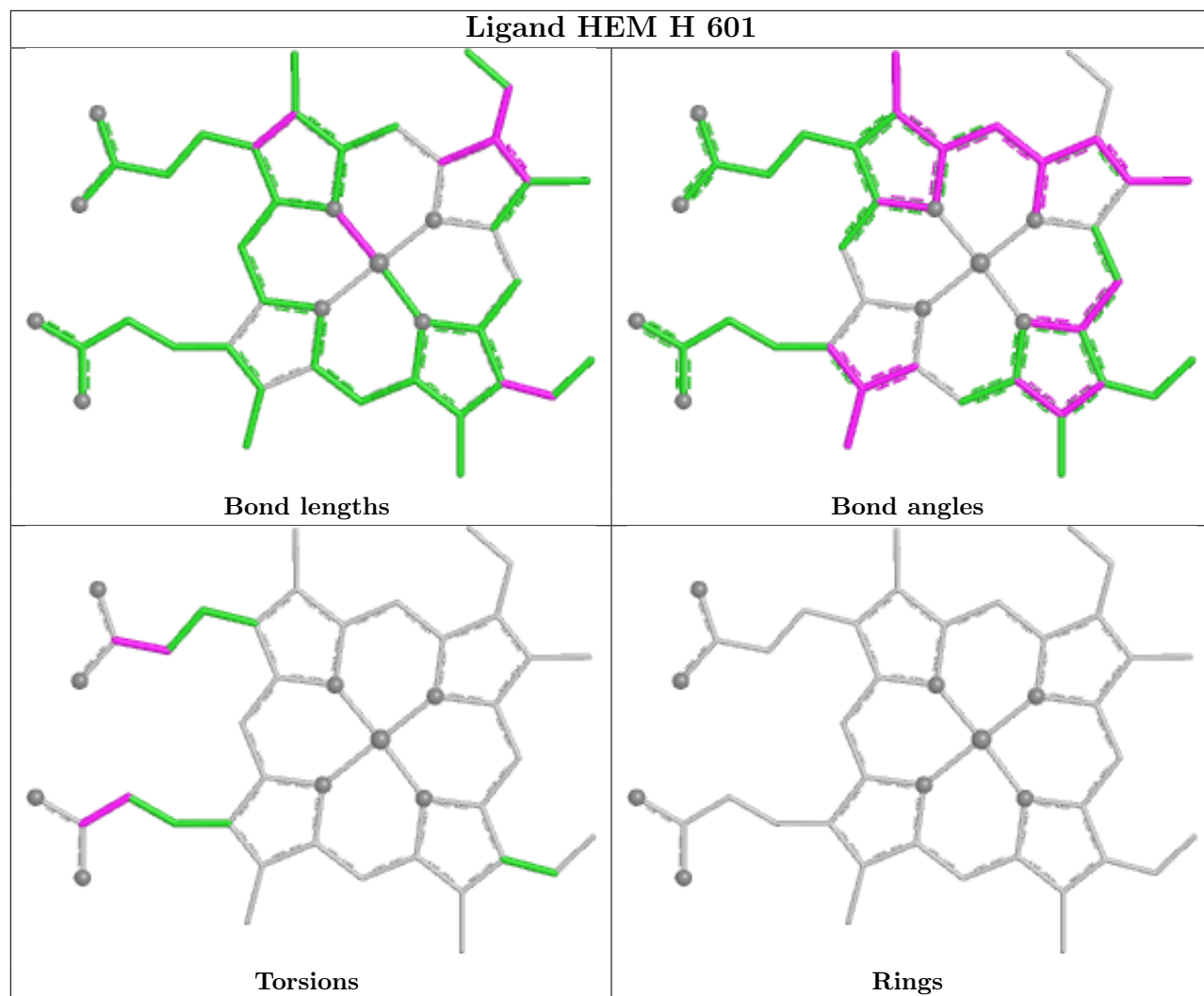


Ligand HEM D 601

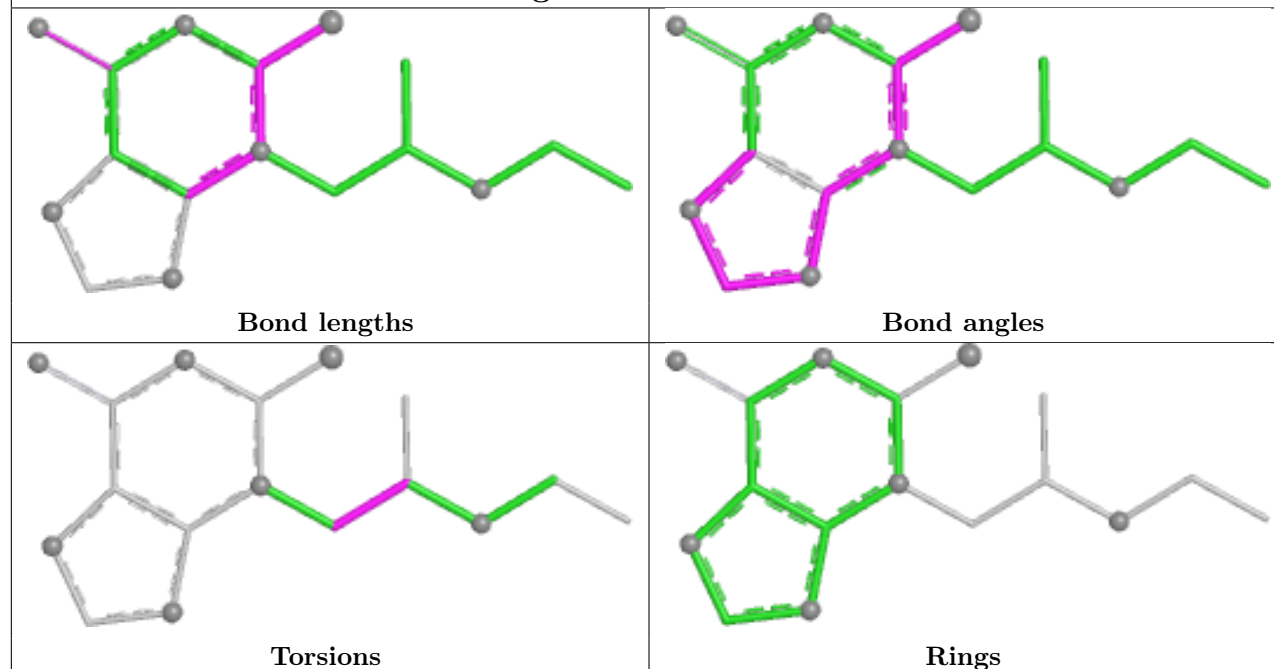




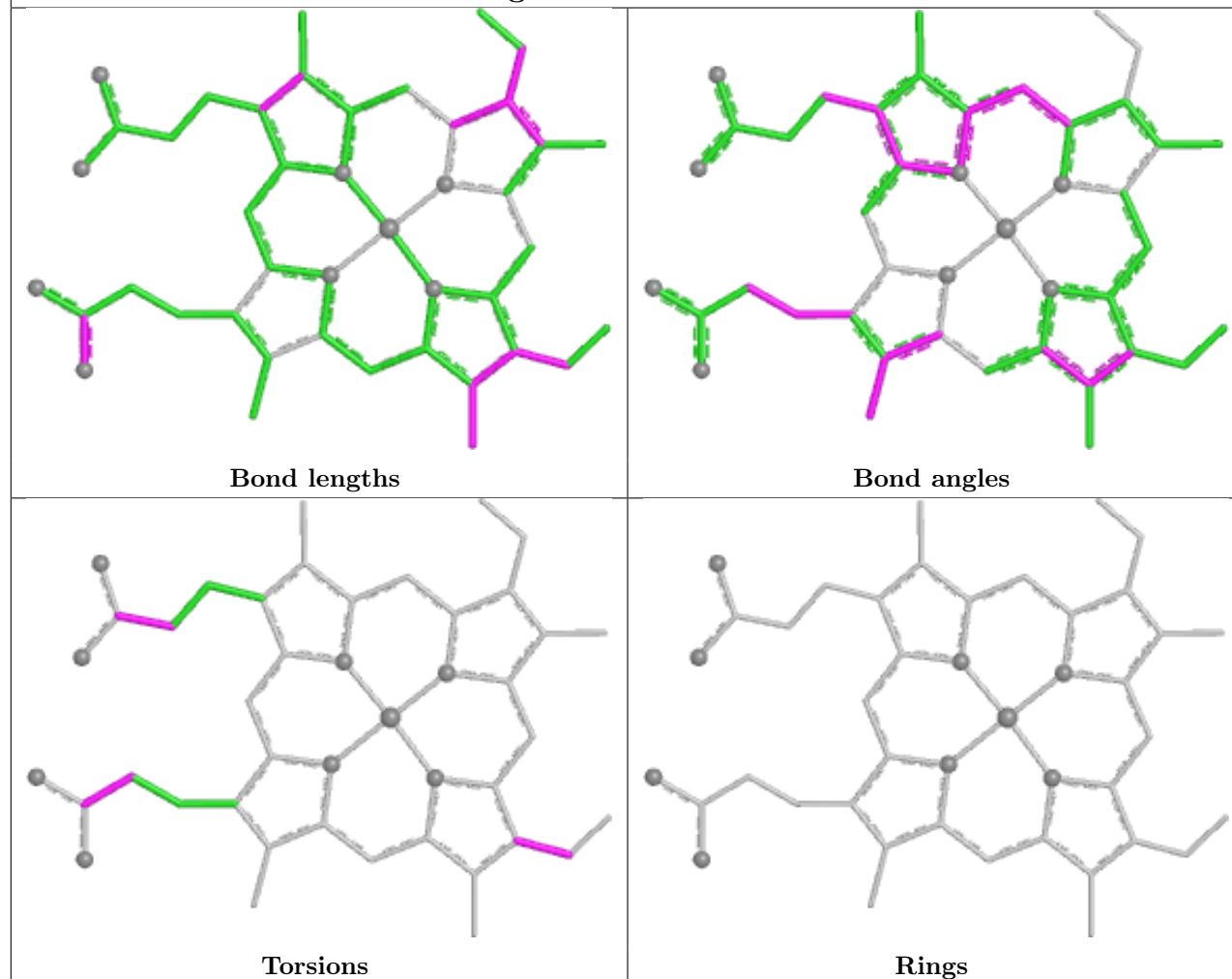


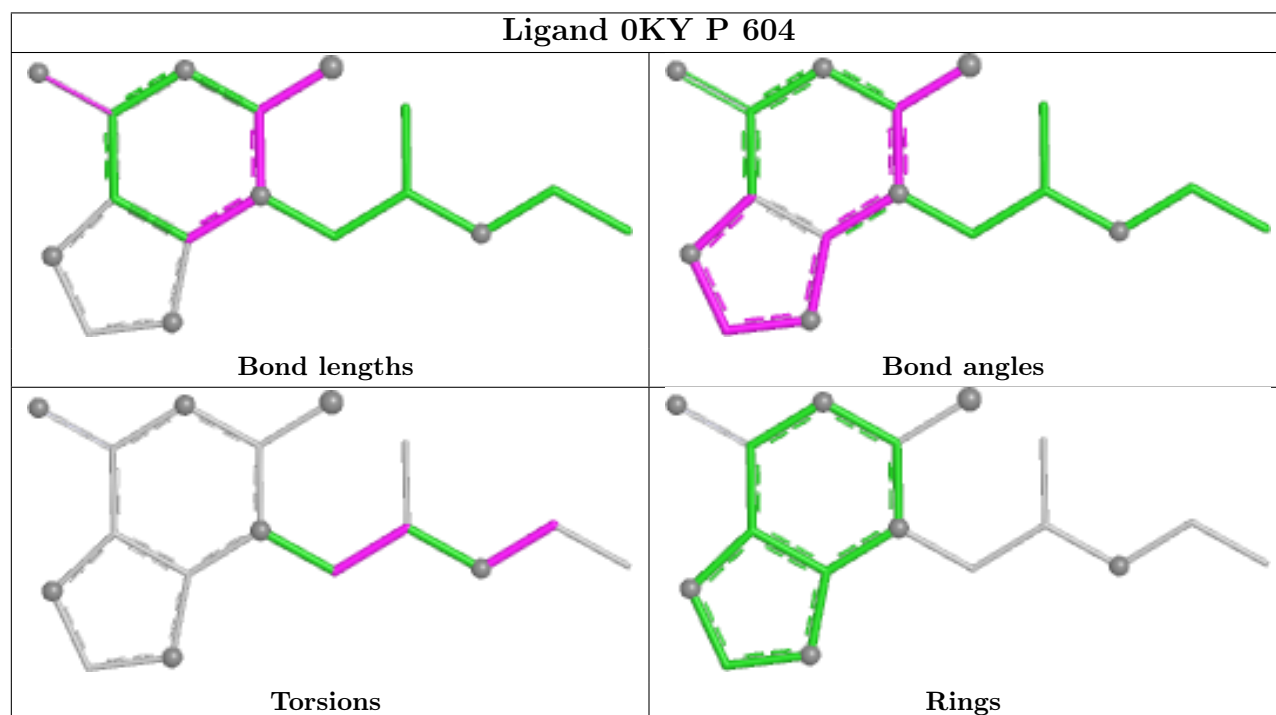
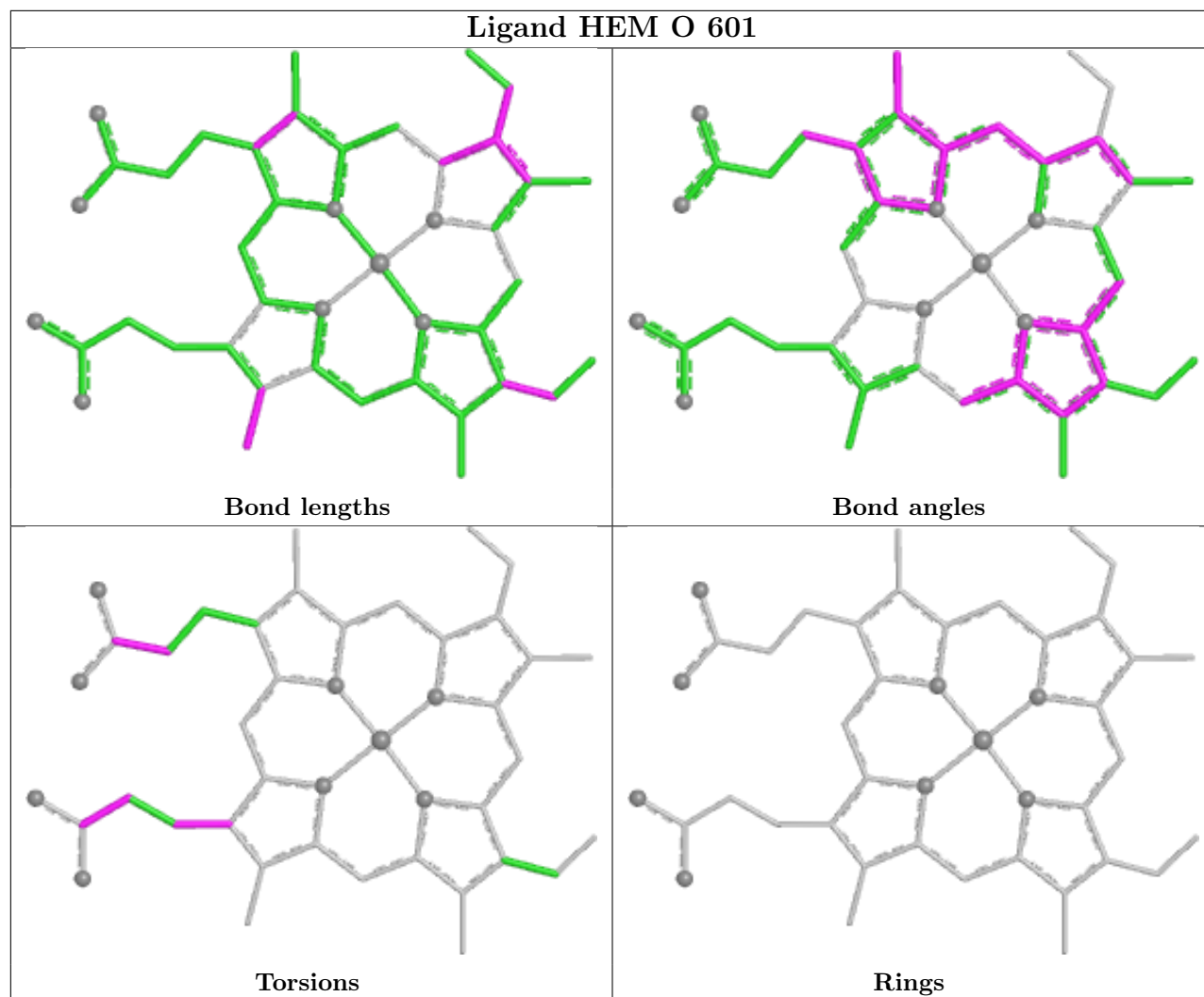


Ligand OKY O 605

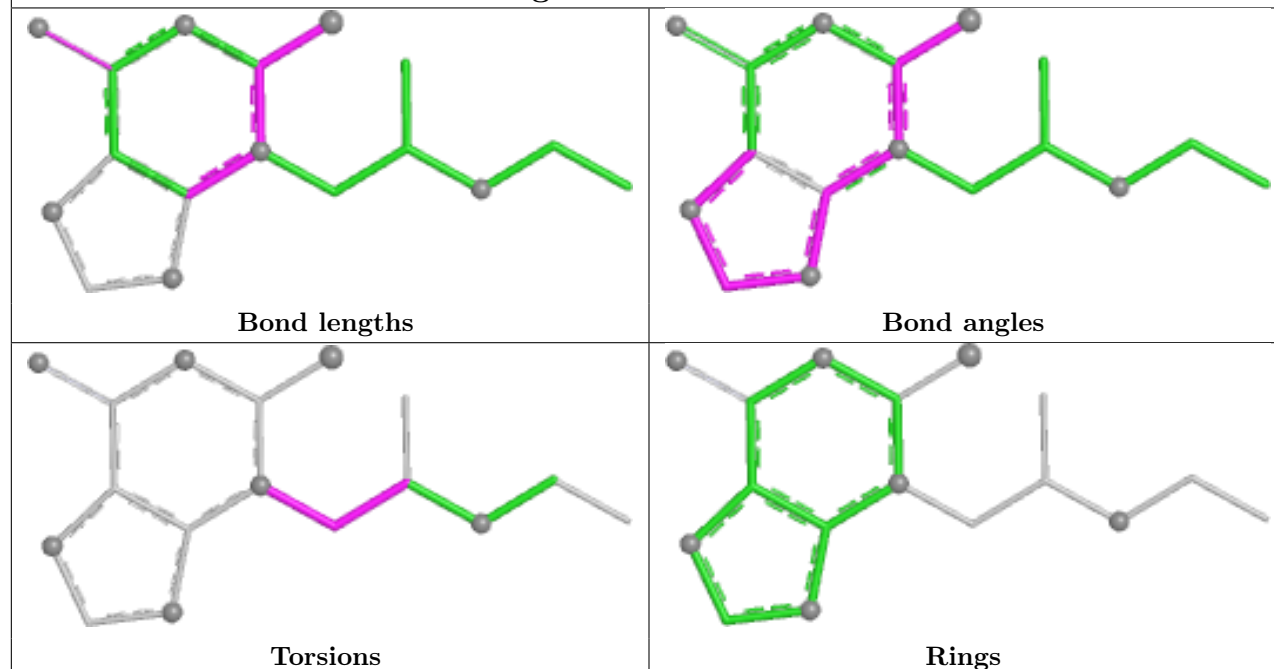


Ligand HEM G 601

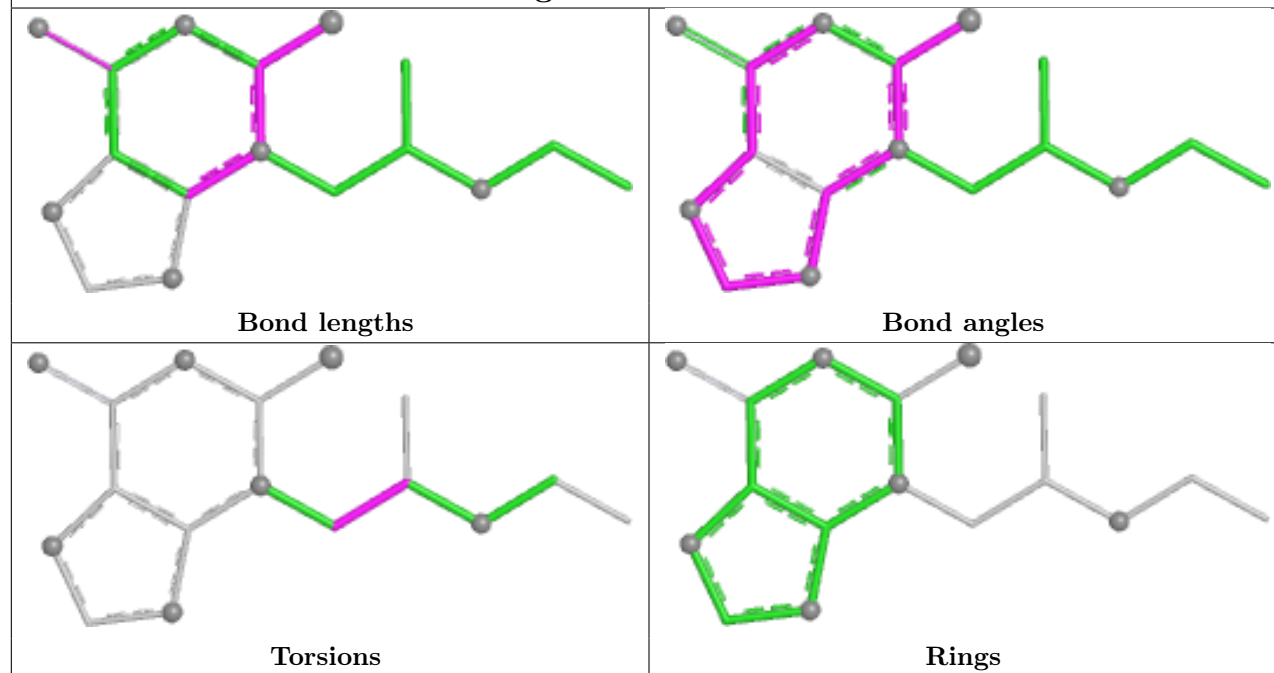


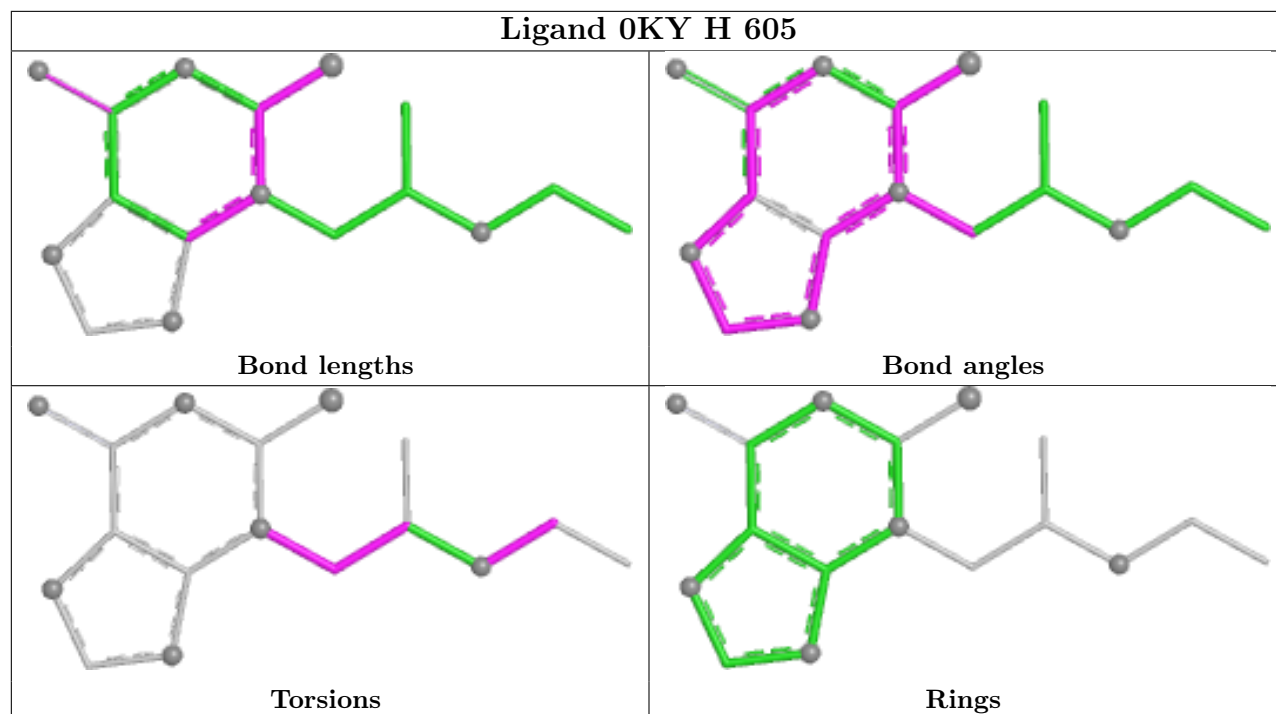


Ligand 0KY K 602



Ligand 0KY L 602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^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

Continued on next page...

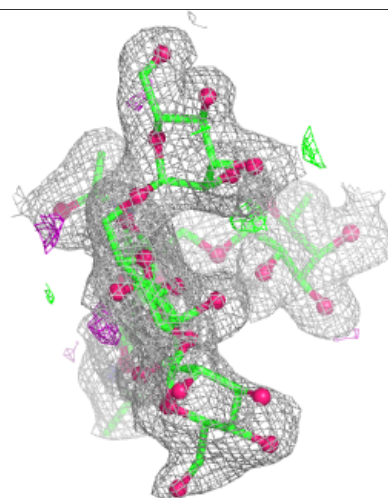
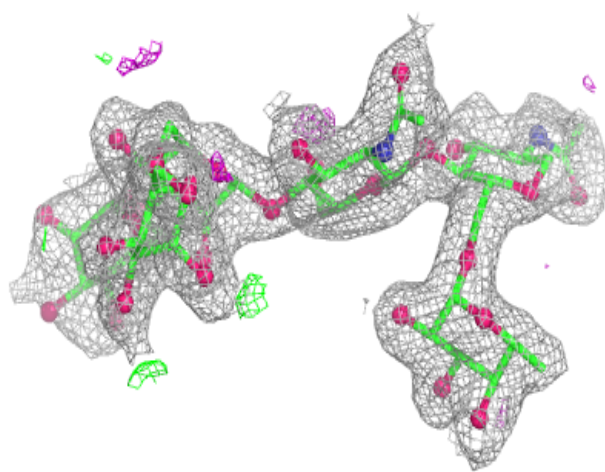
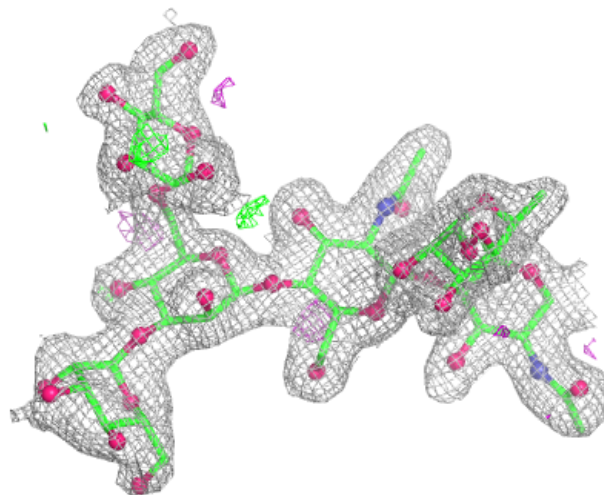
Continued from previous page...

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

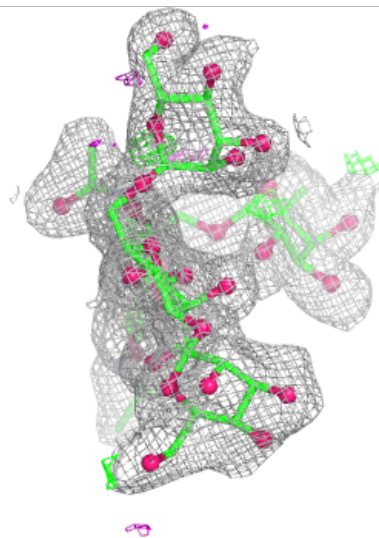
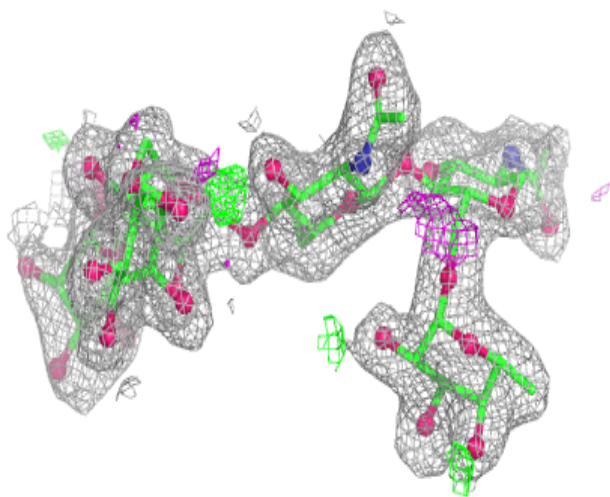
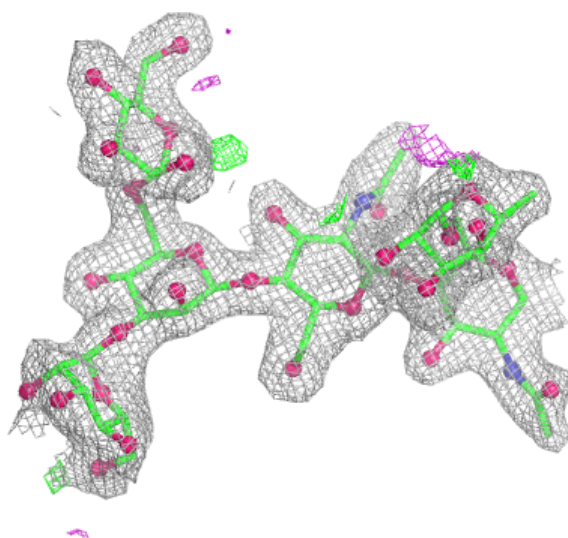
Electron density around Chain Q:

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



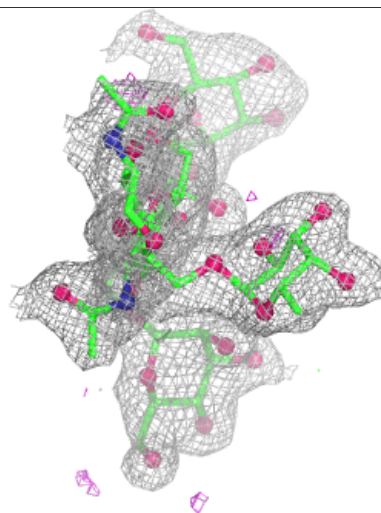
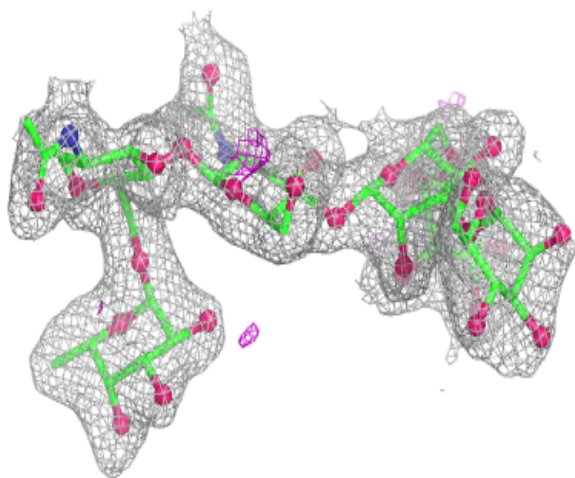
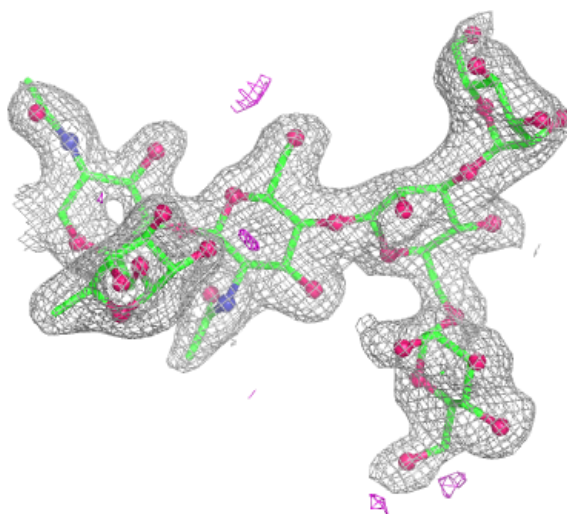
Electron density around Chain R:

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



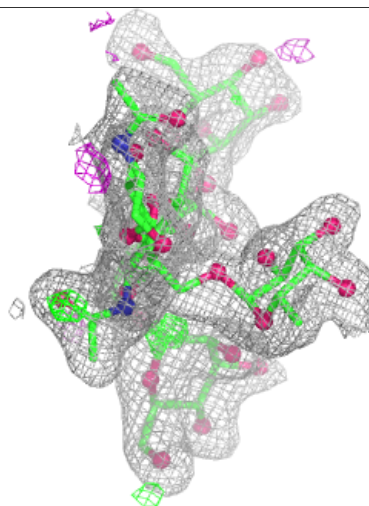
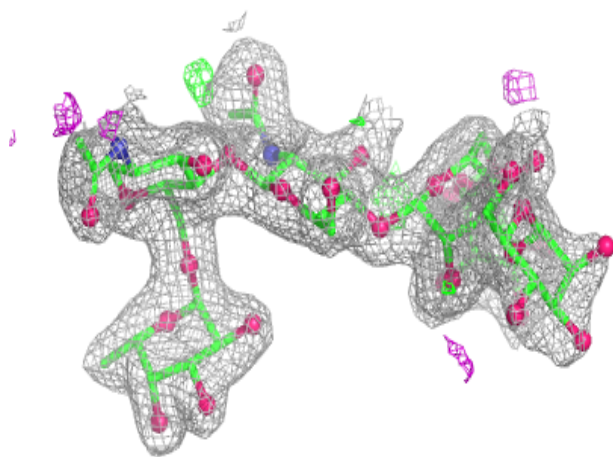
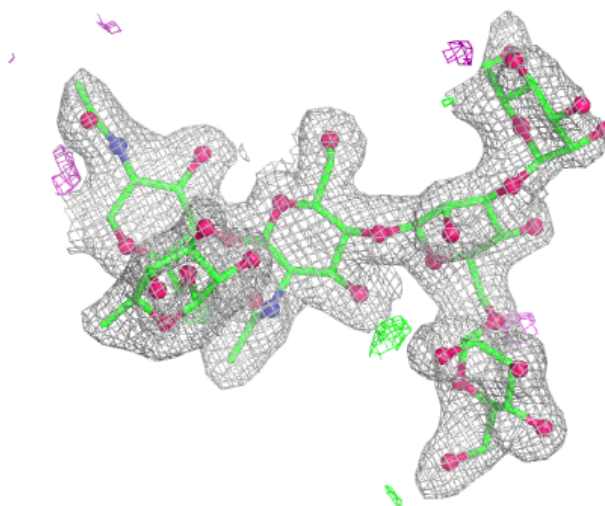
Electron density around Chain S:

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



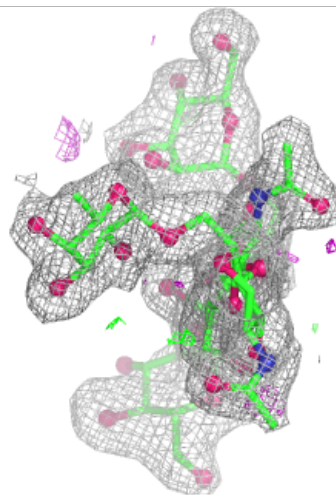
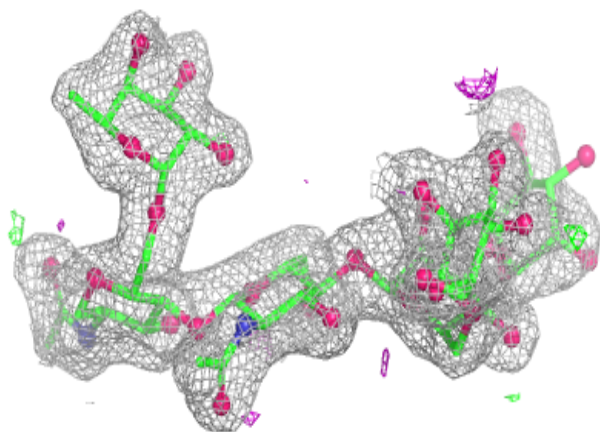
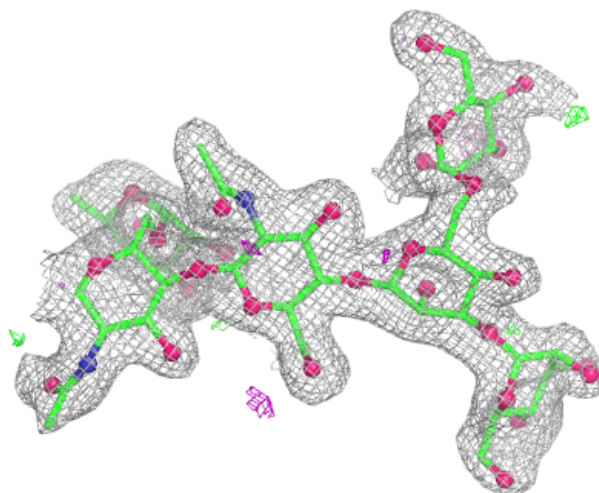
Electron density around Chain T:

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



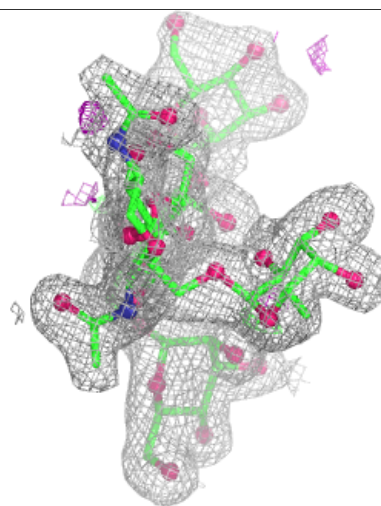
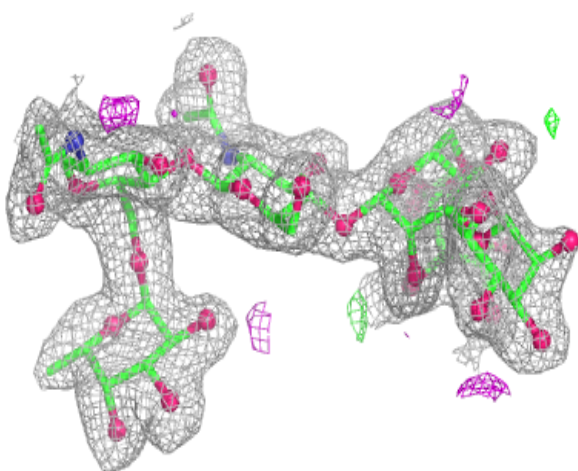
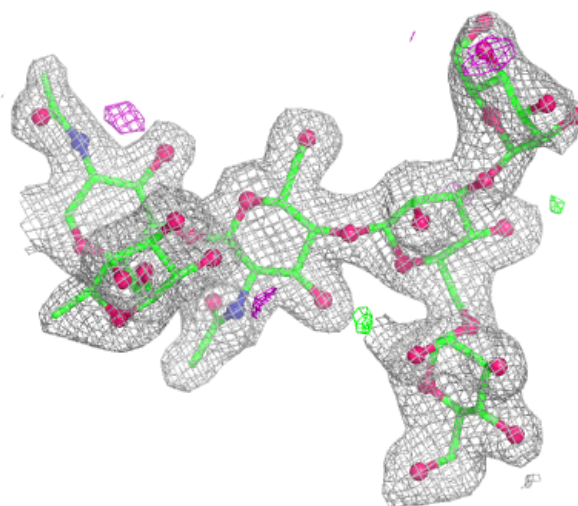
Electron density around Chain U:

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



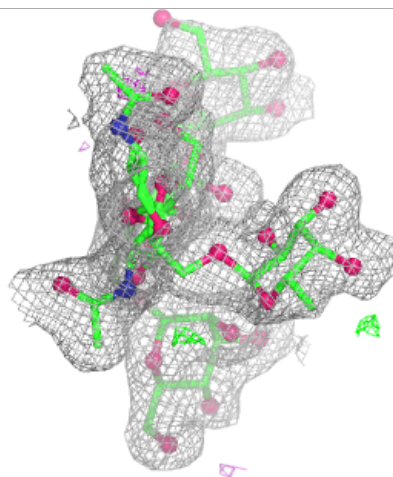
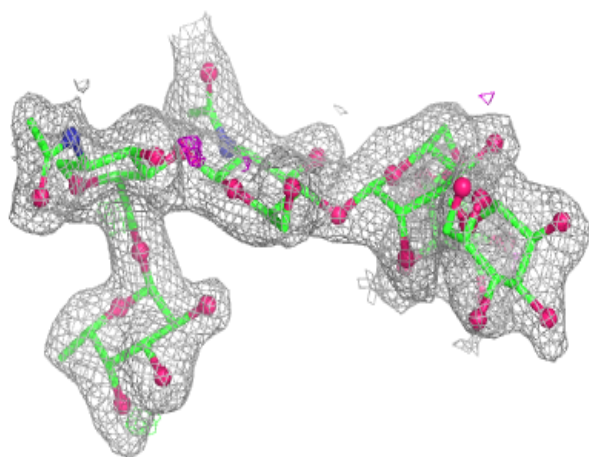
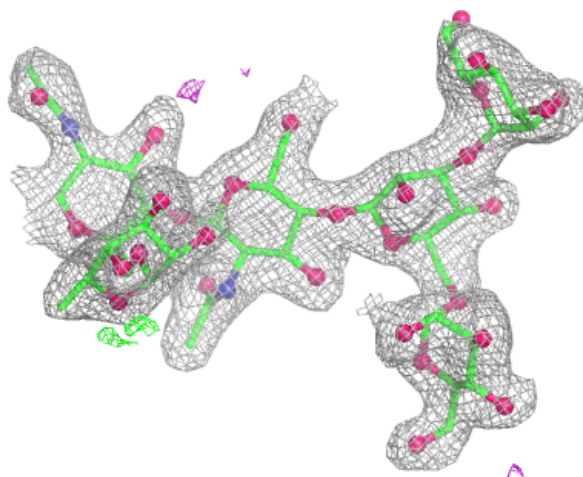
Electron density around Chain V:

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



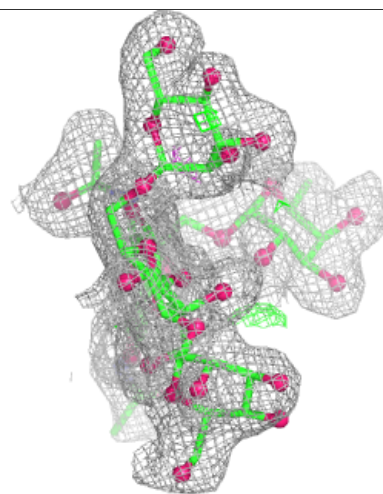
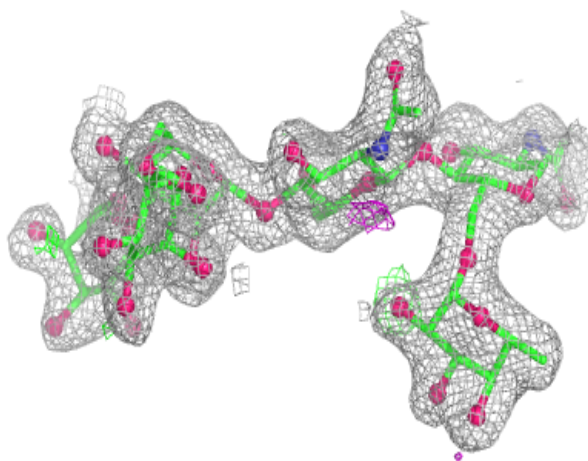
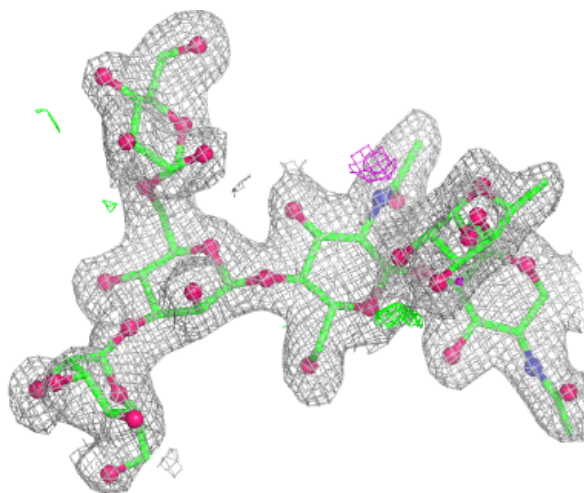
Electron density around Chain W:

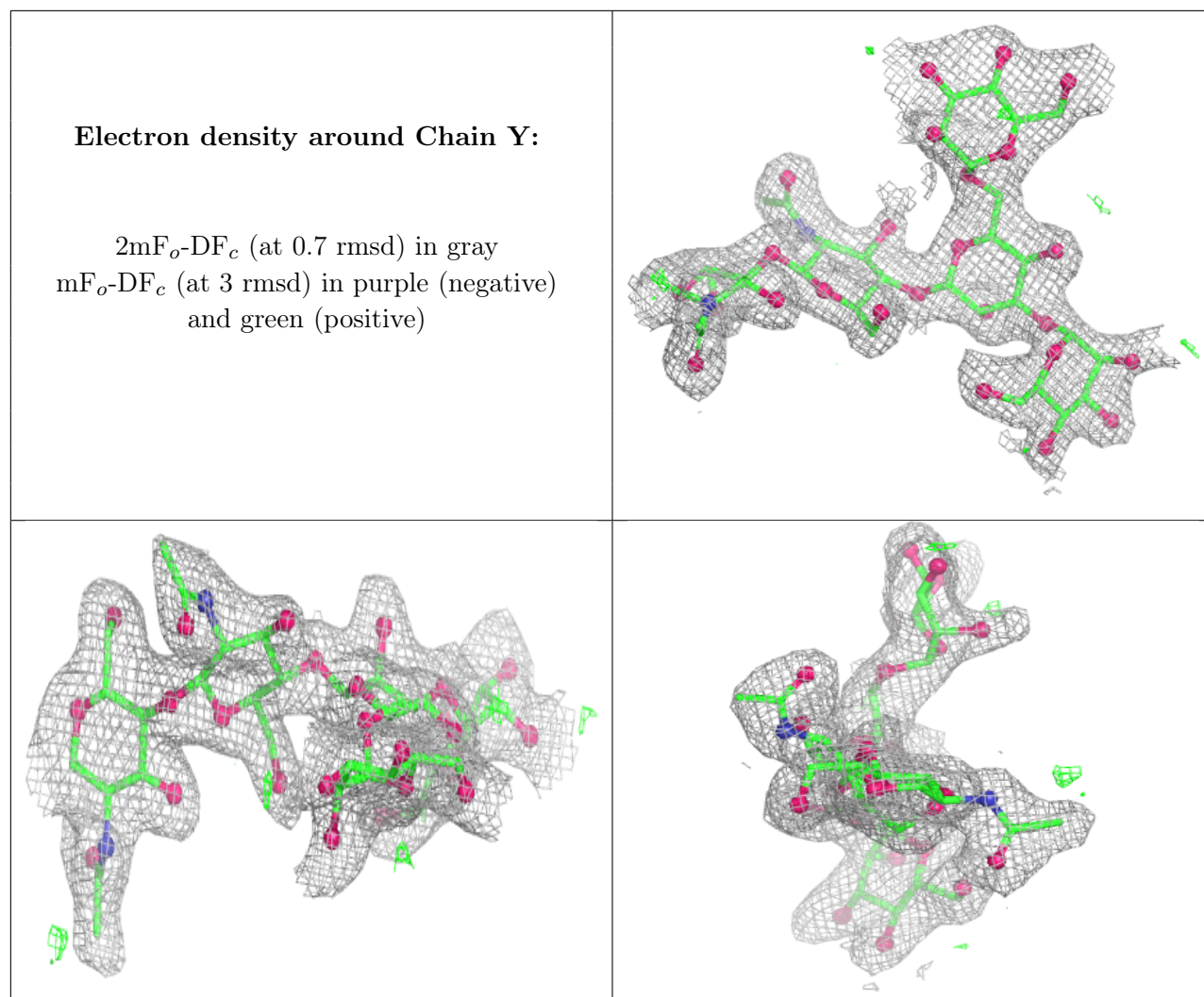
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	O	603	14/15	0.97	0.06	71,75,81,84	0
6	OKY	G	605	17/17	0.98	0.05	38,53,62,62	0
6	OKY	H	605	17/17	0.98	0.06	52,67,75,75	0
6	OKY	K	602	17/17	0.98	0.06	43,59,63,64	0
6	OKY	L	602	17/17	0.98	0.05	50,61,68,68	0
6	OKY	O	605	17/17	0.98	0.06	53,61,70,70	0
6	OKY	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

Continued on next page...

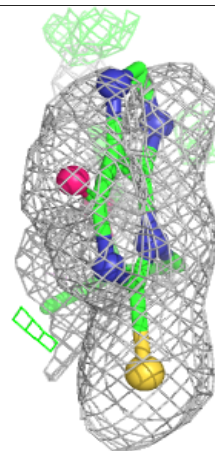
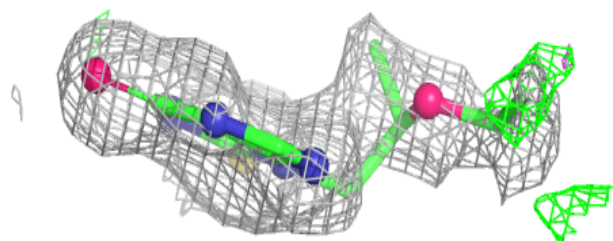
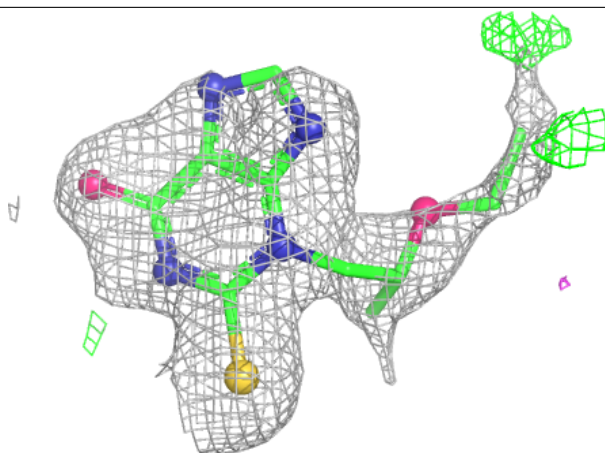
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^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	OKY	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	OKY	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.

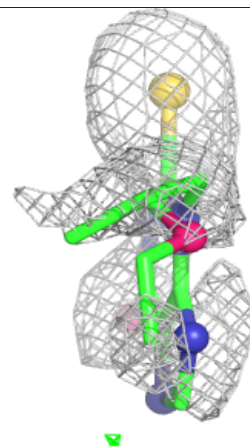
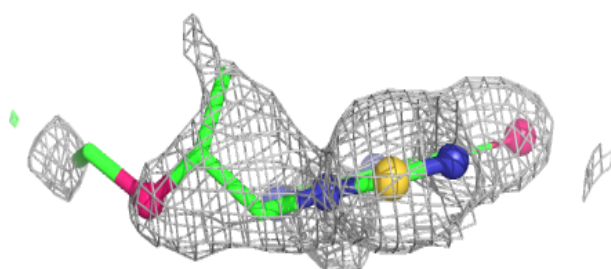
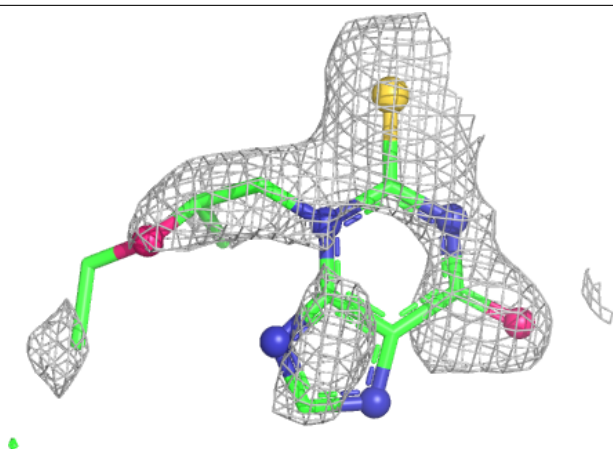
Electron density around 0KY G 605:

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



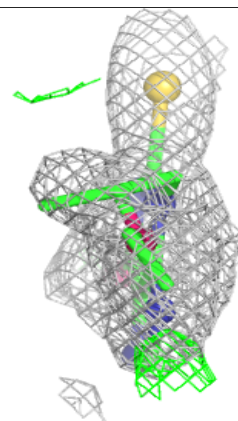
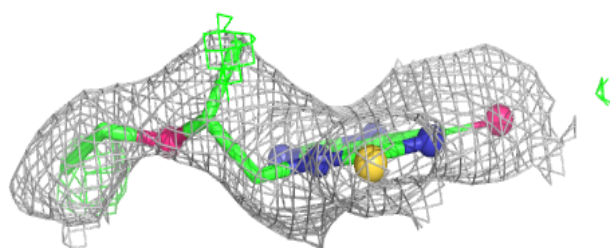
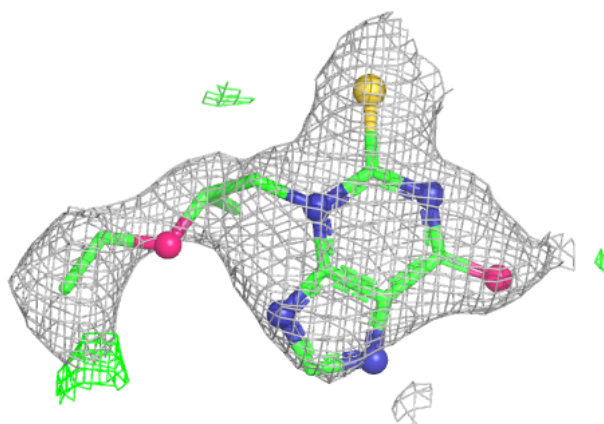
Electron density around 0KY H 605:

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



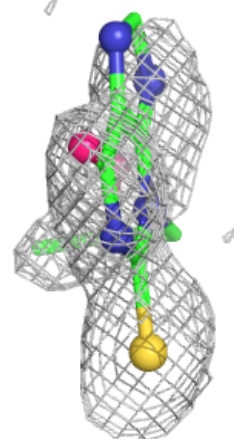
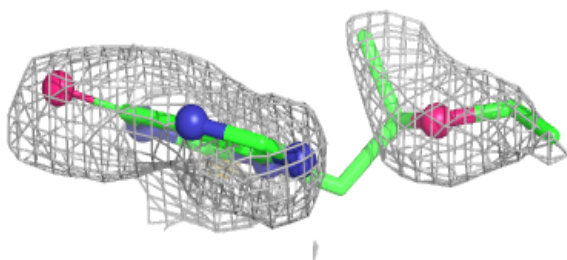
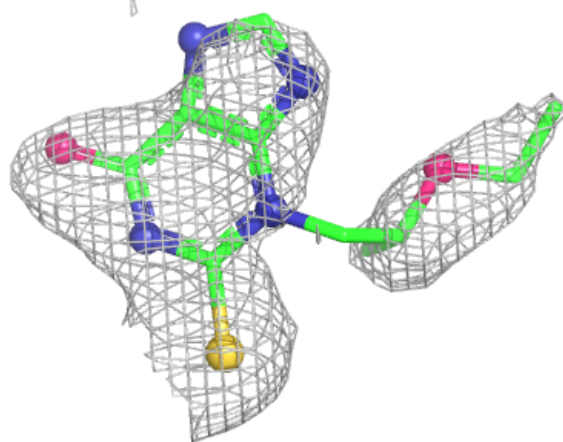
Electron density around 0KY K 602:

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



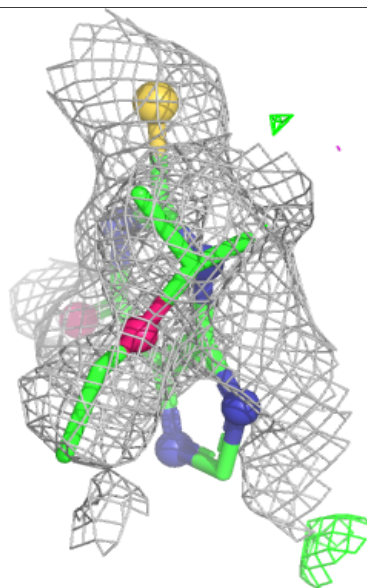
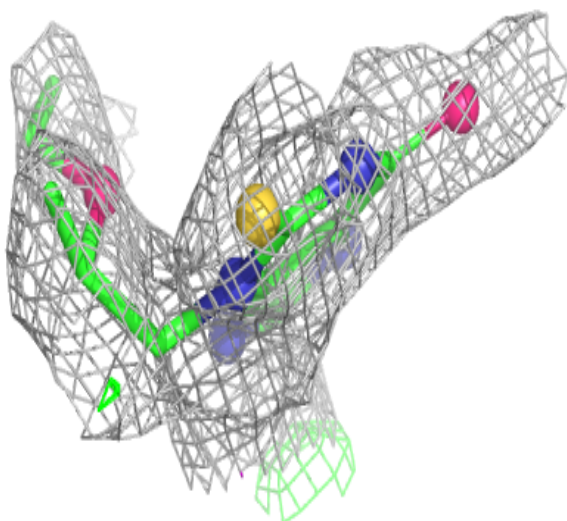
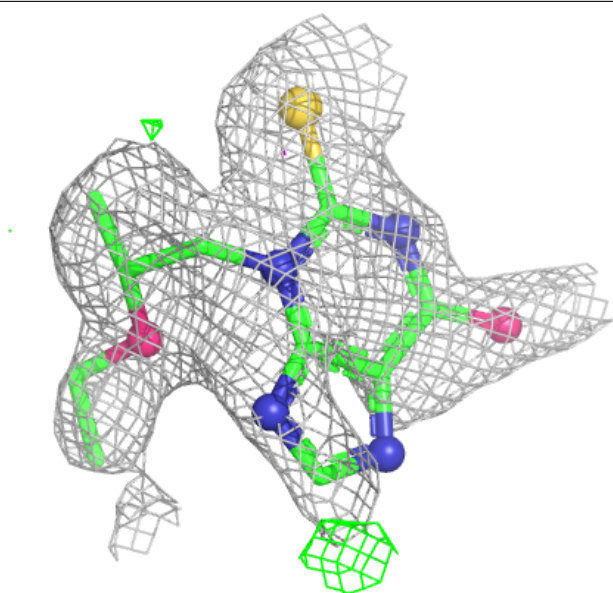
Electron density around 0KY L 602:

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



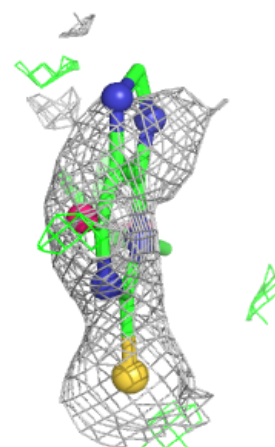
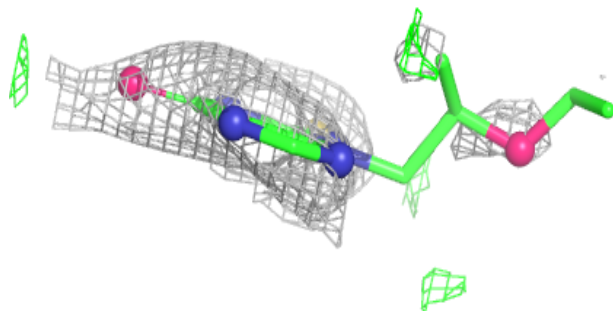
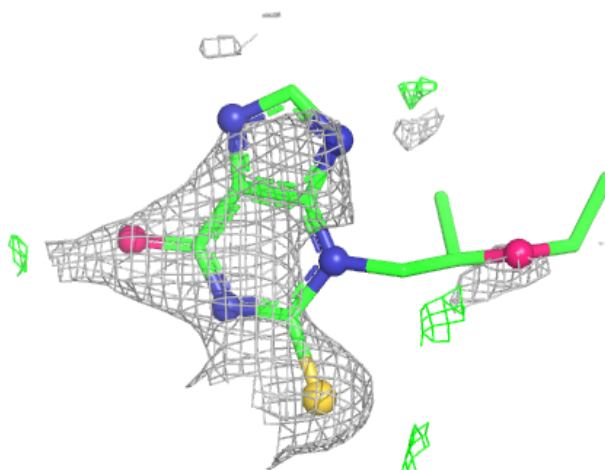
Electron density around 0KY O 605:

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



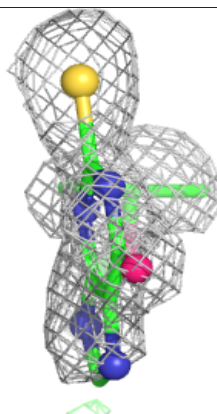
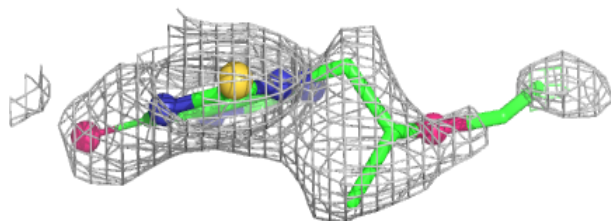
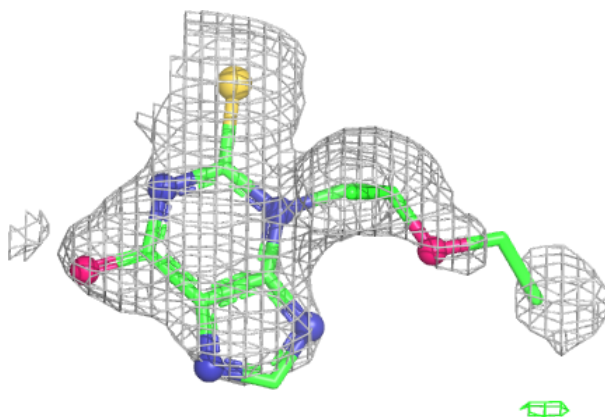
Electron density around 0KY P 604:

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



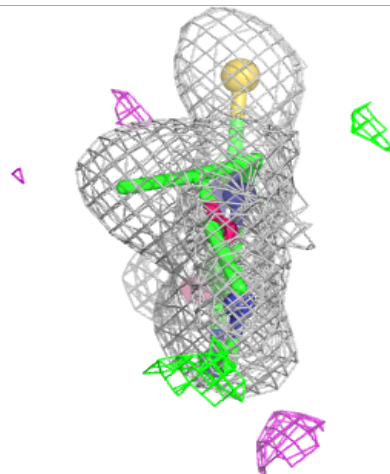
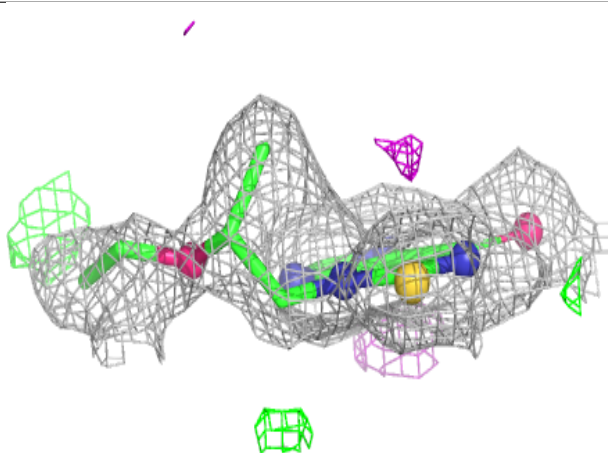
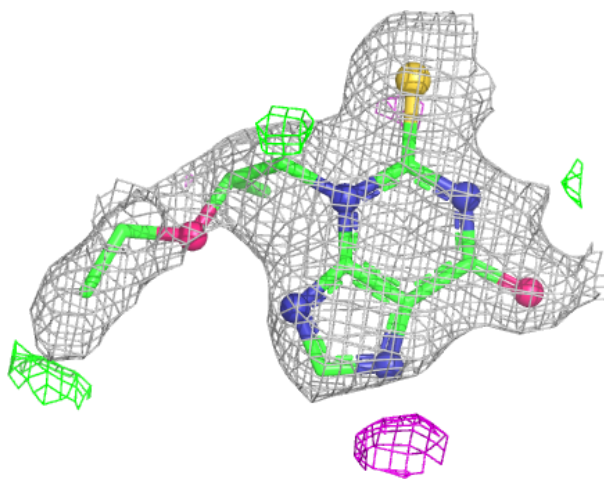
Electron density around 0KY D 602:

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



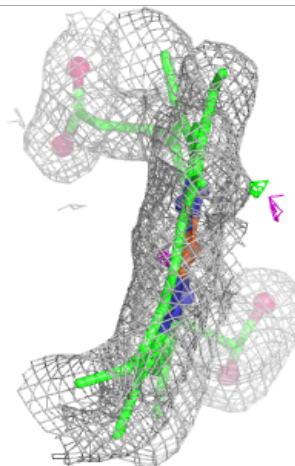
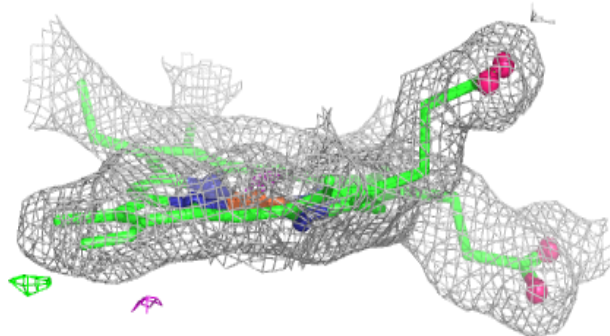
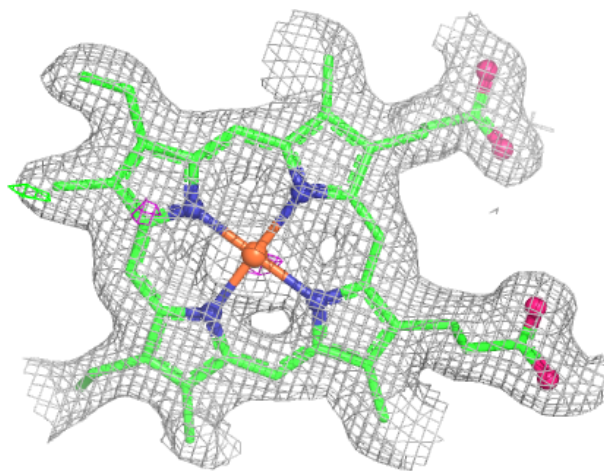
Electron density around 0KY C 601:

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



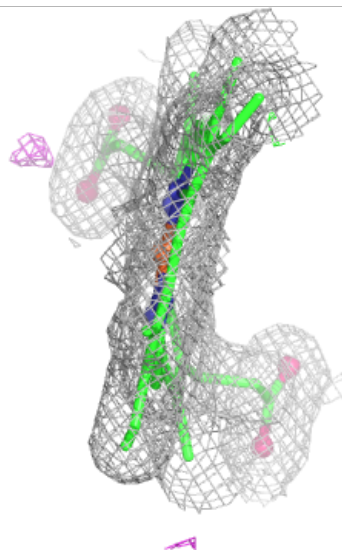
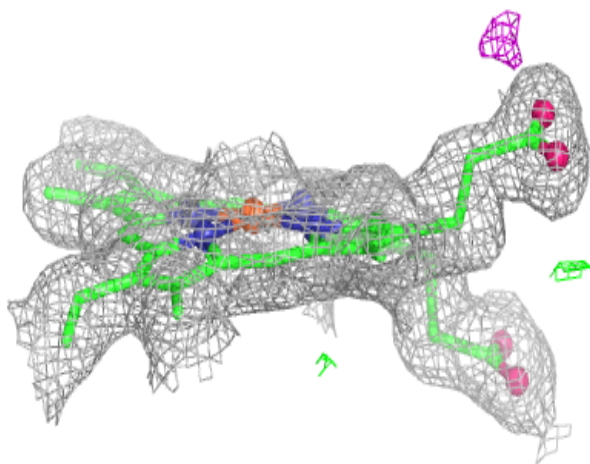
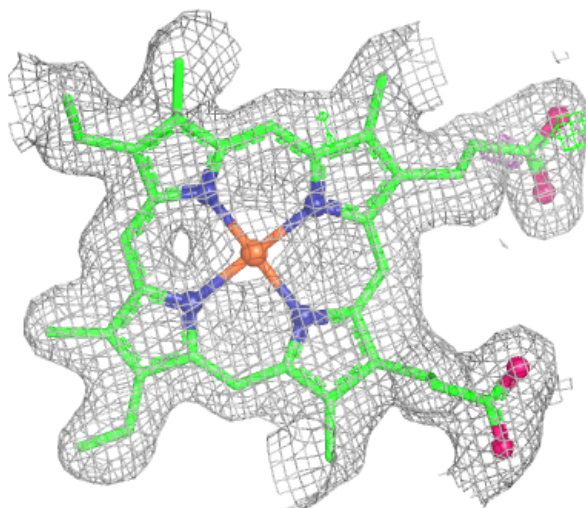
Electron density around HEM L 601:

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



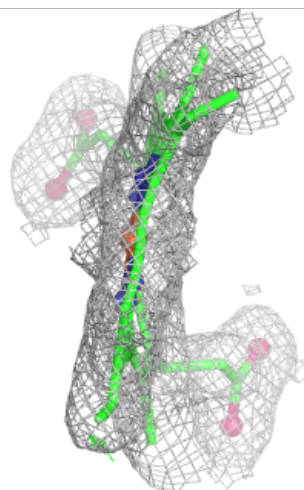
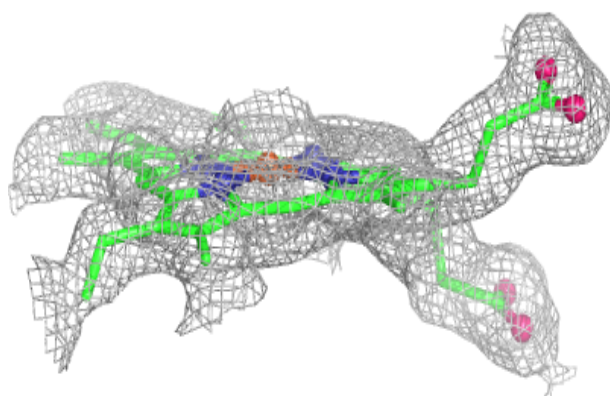
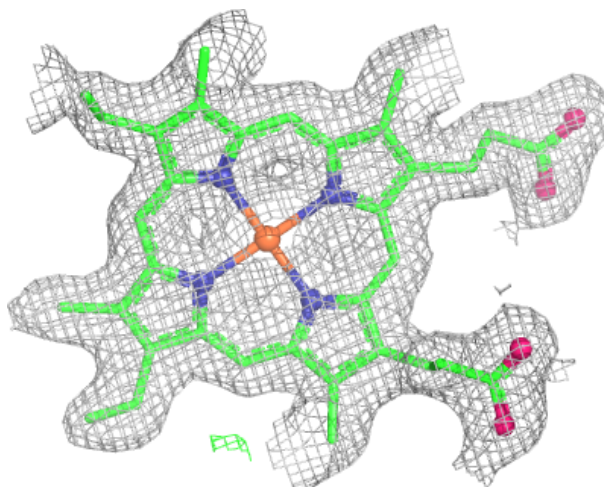
Electron density around HEM C 602:

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



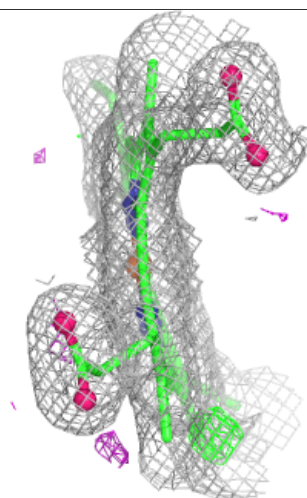
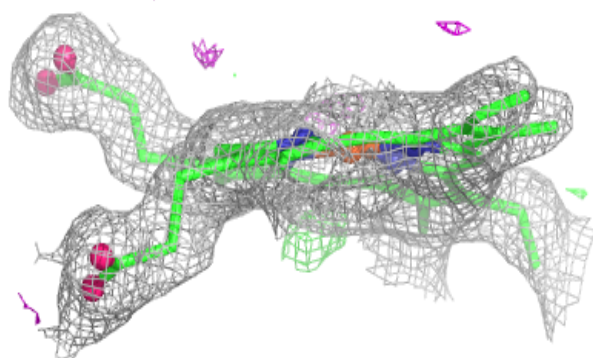
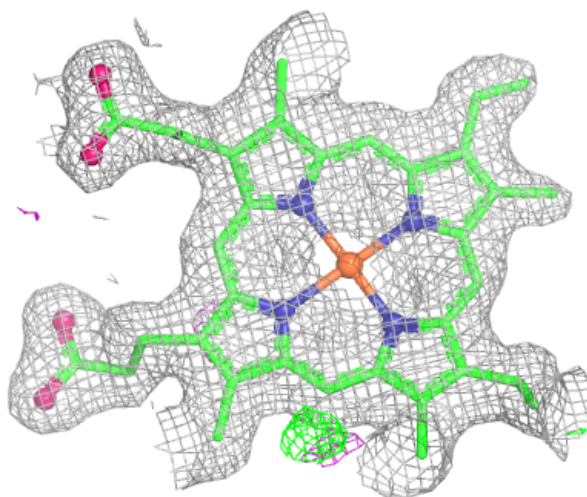
Electron density around HEM D 601:

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



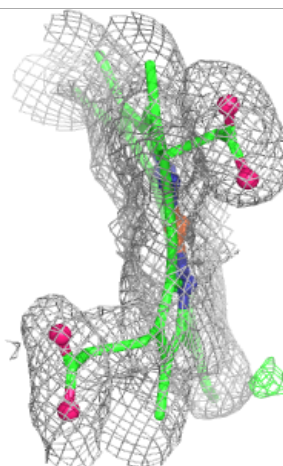
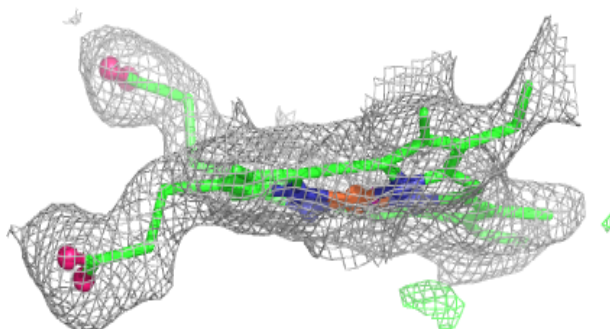
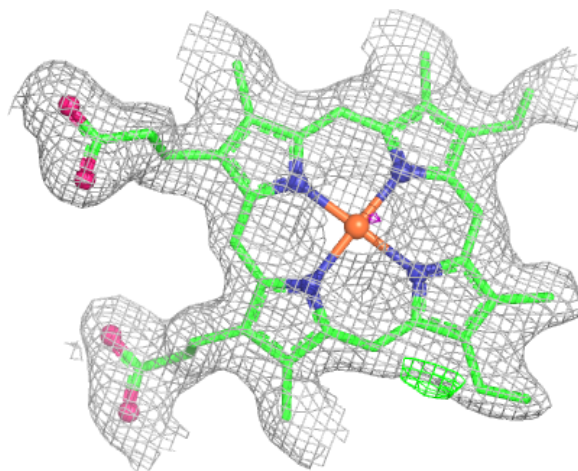
Electron density around HEM G 601:

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



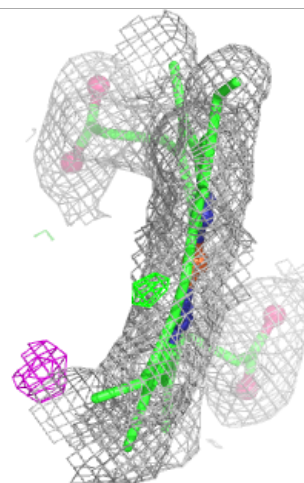
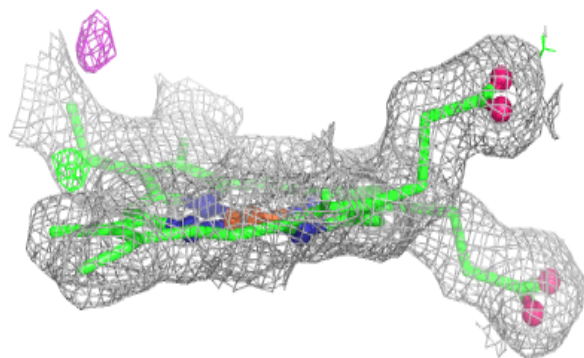
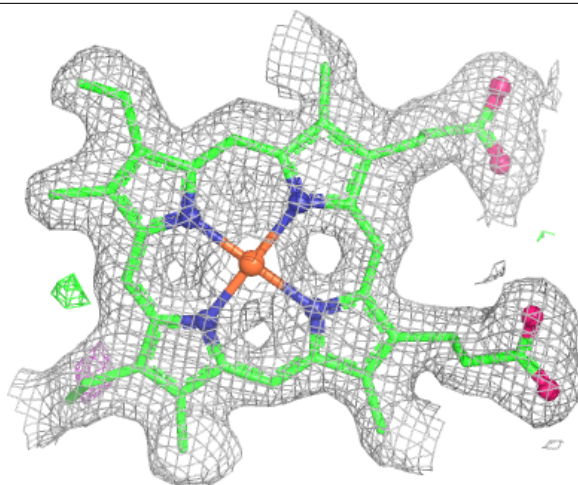
Electron density around HEM H 601:

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



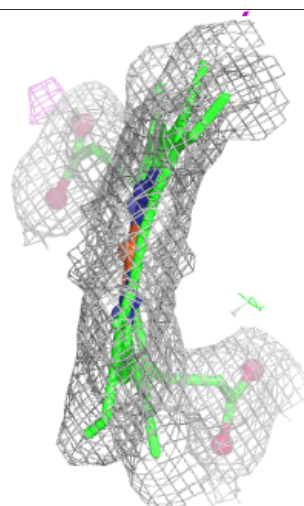
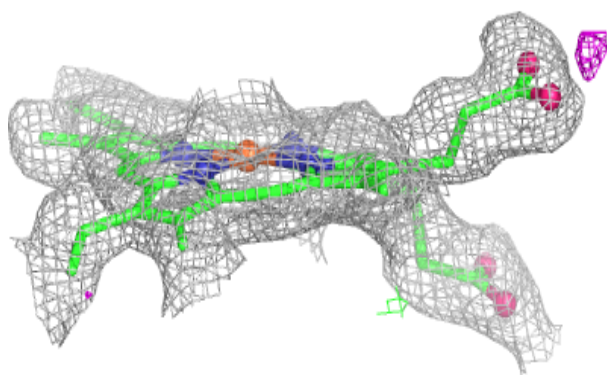
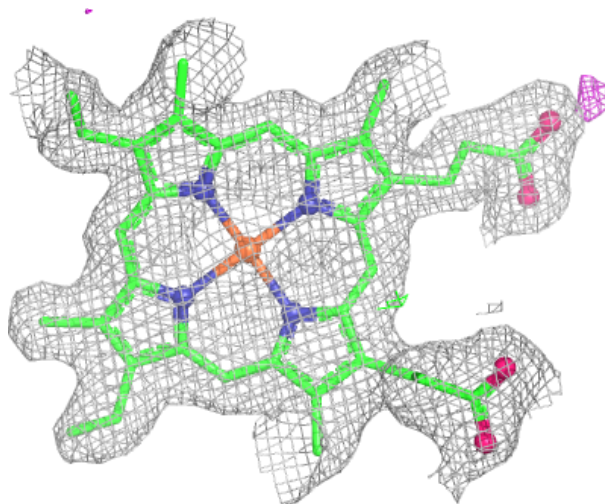
Electron density around HEM K 601:

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



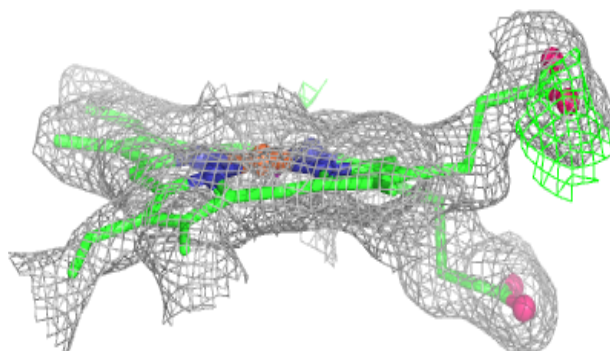
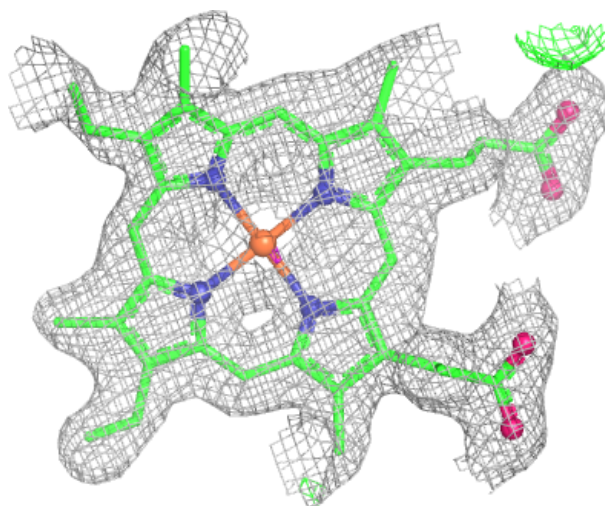
Electron density around HEM O 601:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.