Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 05:08 AM EST

PDB ID	:	4F4O
Title	:	Structure of the Haptoglobin-Haemoglobin Complex
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Deposited on	:	2012-05-11
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

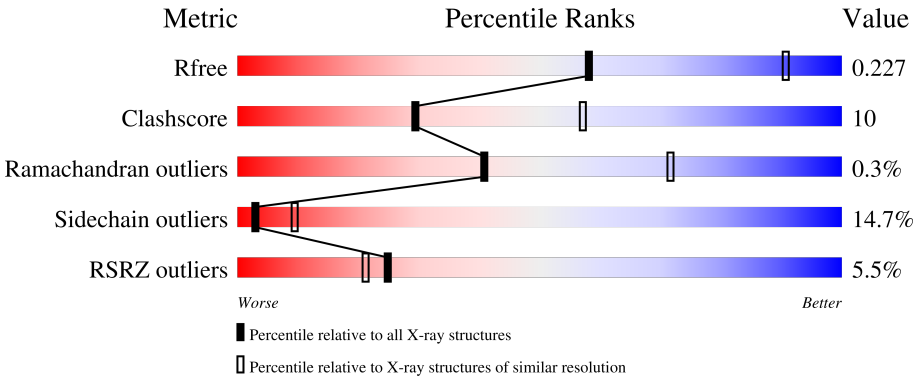
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	141	82% 15% ·
1	D	141	81% 16% ·
1	G	141	84% 13% ·
1	J	141	23% 79% 18% ·
2	B	146	75% 22% ·

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Mol	Chain	Length	Quality of chain
2	E	146	5% 73% 23%
2	H	146	% 75% 22%
2	K	146	43% 68% 24% 8%
3	C	347	2% 58% 27% 5% 11%
3	F	347	2% 61% 24% 5% 11%
3	I	347	59% 26% 11%
3	L	347	3% 59% 25% 5% 11%
4	M	2	100%
4	O	2	100%
4	Q	2	100%
5	N	2	100%
5	P	2	50% 50%
5	R	2	100%
5	S	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	P	1	-	-	-	X
5	FUC	P	2	-	-	-	X
8	NAG	C	1003	-	-	-	X
8	NAG	F	1003	-	-	-	X
8	NAG	I	1003	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 19196 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 Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			
1	D	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			
1	G	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			
1	J	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	1	0
			1144	731	205	206	2			
2	E	146	Total	C	N	O	S	0	1	0
			1144	731	205	206	2			
2	H	146	Total	C	N	O	S	0	1	0
			1144	731	205	206	2			
2	K	146	Total	C	N	O	S	0	1	0
			1144	731	205	206	2			

- Molecule 3 is a protein called Haptoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	309	Total	C	N	O	S	0	0	0
			2428	1546	411	457	14			
3	F	309	Total	C	N	O	S	0	0	0
			2428	1546	411	457	14			
3	I	309	Total	C	N	O	S	0	0	0
			2428	1546	411	457	14			
3	L	309	Total	C	N	O	S	0	0	0
			2428	1546	411	457	14			

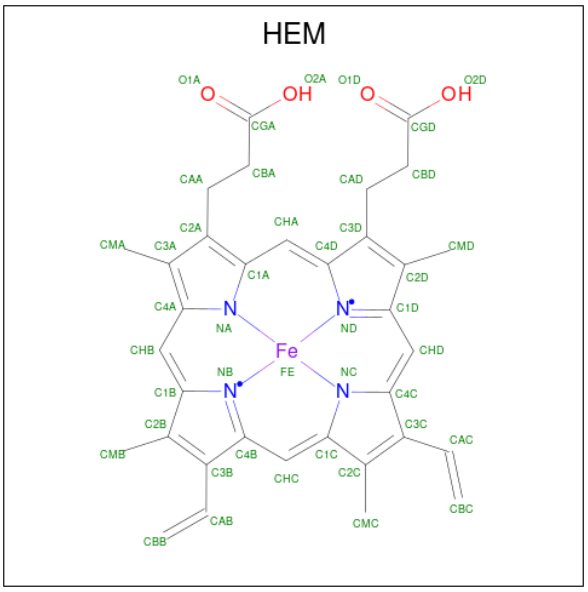
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

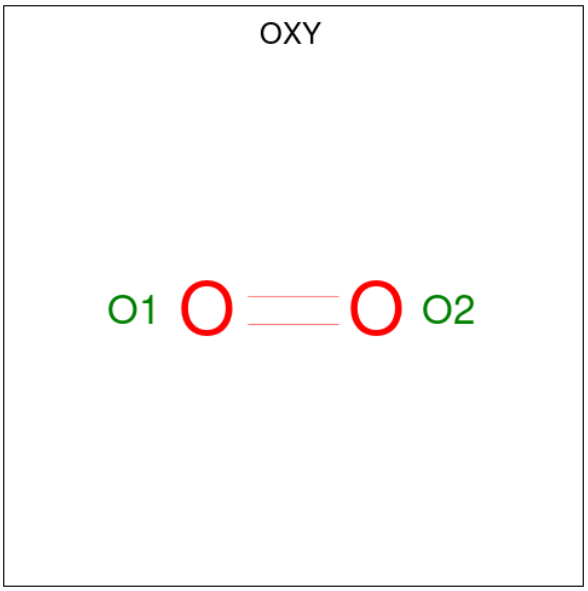
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	N	2	Total	C	N	O	0	0	0
			24	14	1	9			
5	P	2	Total	C	N	O	0	0	0
			24	14	1	9			
5	R	2	Total	C	N	O	0	0	0
			24	14	1	9			
5	S	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



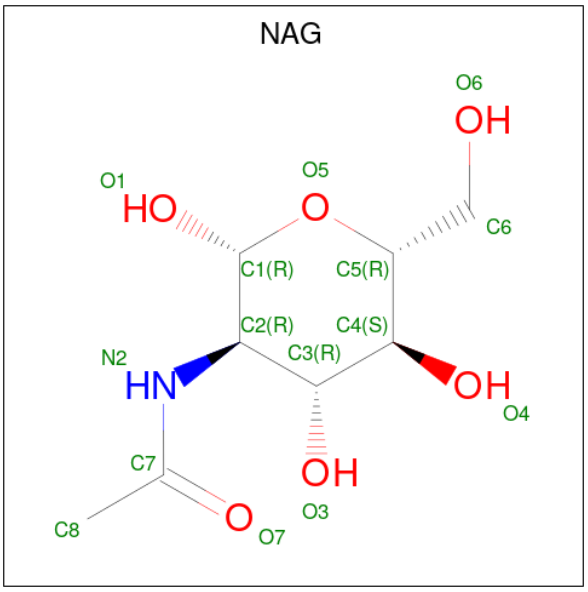
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 7 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 2 2	0	0
7	B	1	Total O 2 2	0	0
7	D	1	Total O 2 2	0	0
7	E	1	Total O 2 2	0	0
7	G	1	Total O 2 2	0	0
7	H	1	Total O 2 2	0	0
7	J	1	Total O 2 2	0	0
7	K	1	Total O 2 2	0	0

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



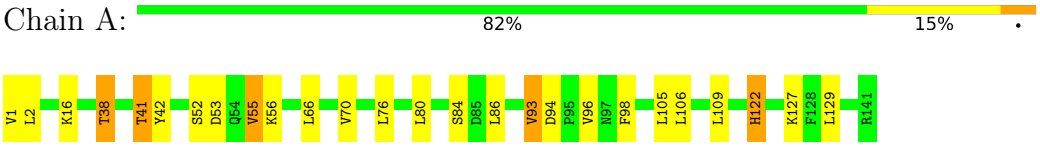
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C N O 14 8 1 5	0	0
8	C	1	Total C N O 14 8 1 5	0	0
8	F	1	Total C N O 14 8 1 5	0	0
8	F	1	Total C N O 14 8 1 5	0	0
8	I	1	Total C N O 14 8 1 5	0	0
8	I	1	Total C N O 14 8 1 5	0	0
8	L	1	Total C N O 14 8 1 5	0	0
8	L	1	Total C N O 14 8 1 5	0	0

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.

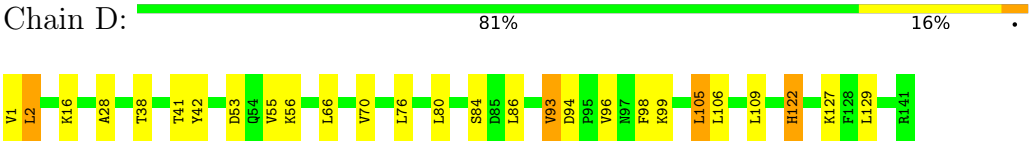
• Molecule 1: Hemoglobin subunit alpha

Chain A:



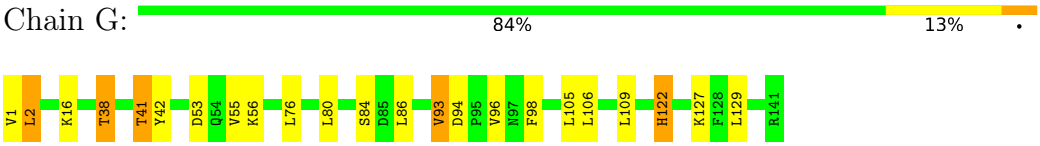
• Molecule 1: Hemoglobin subunit alpha

Chain D:



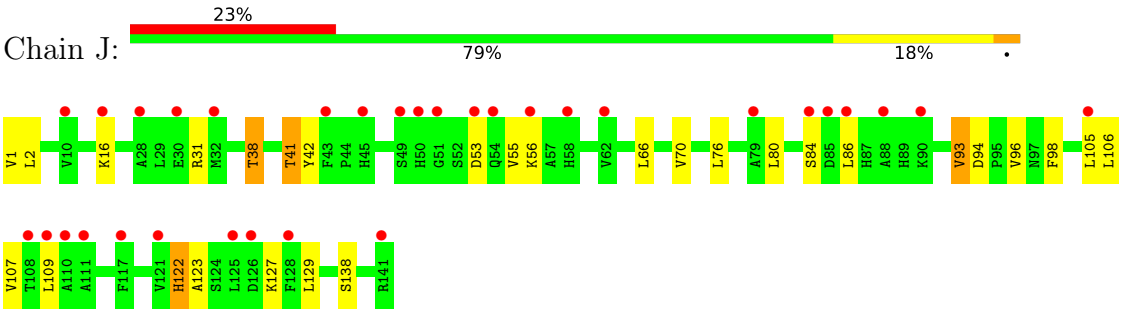
• Molecule 1: Hemoglobin subunit alpha

Chain G:



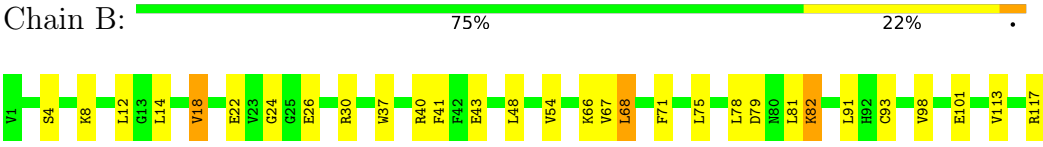
• Molecule 1: Hemoglobin subunit alpha

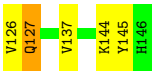
Chain J:



• Molecule 2: Hemoglobin subunit beta

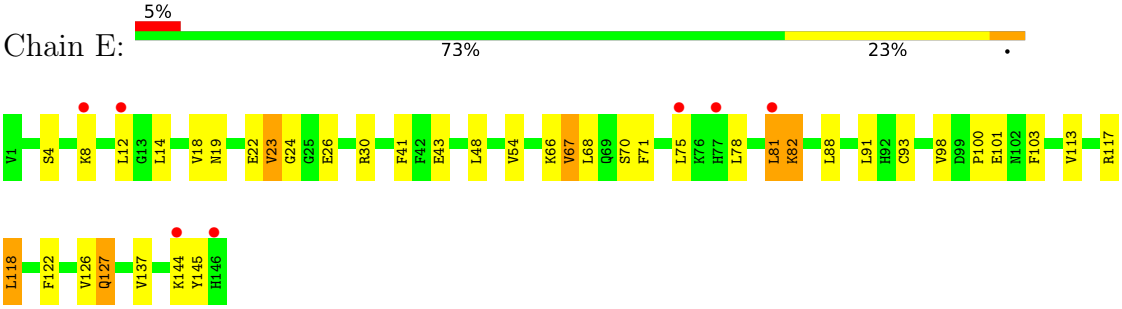
Chain B:





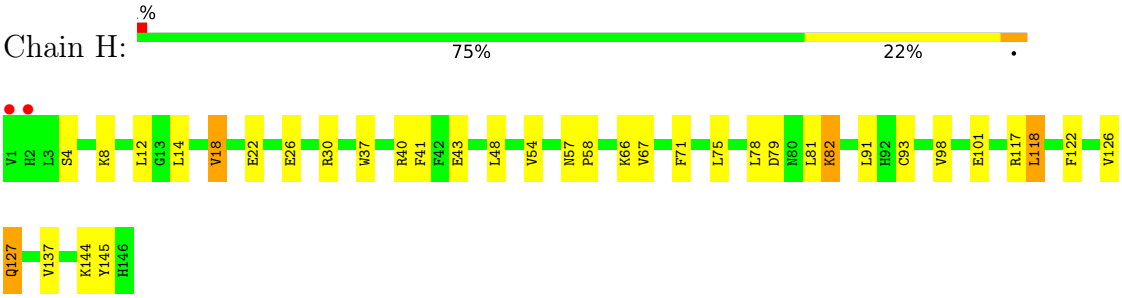
• Molecule 2: Hemoglobin subunit beta

Chain E:



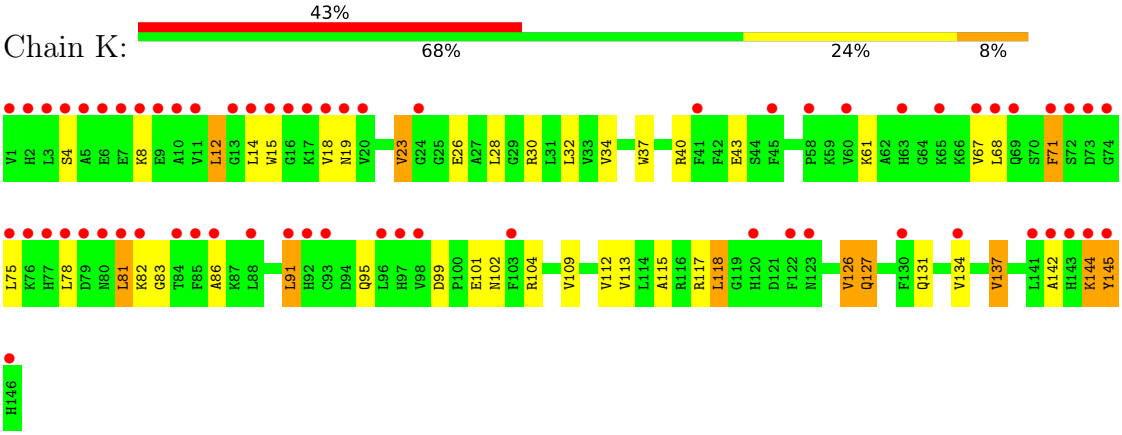
• Molecule 2: Hemoglobin subunit beta

Chain H:



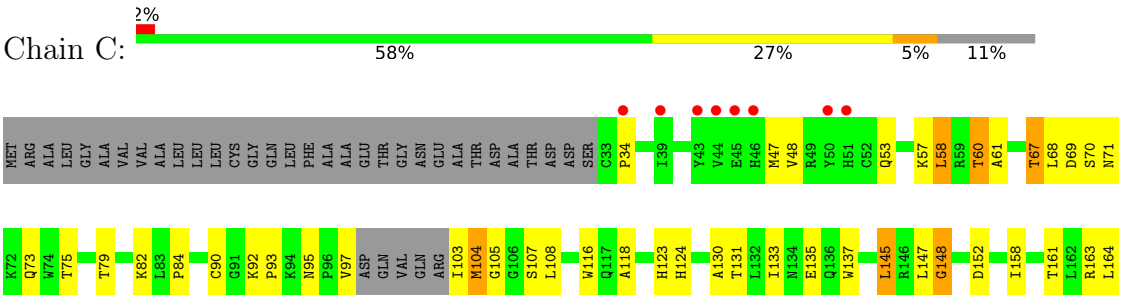
• Molecule 2: Hemoglobin subunit beta

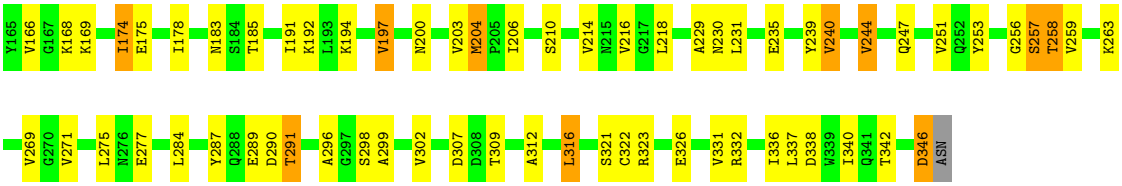
Chain K:



• Molecule 3: Haptoglobin

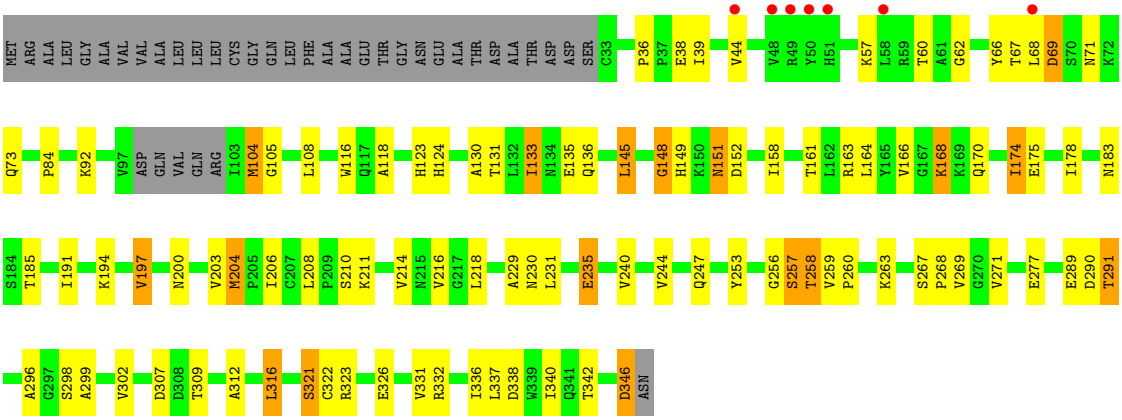
Chain C:





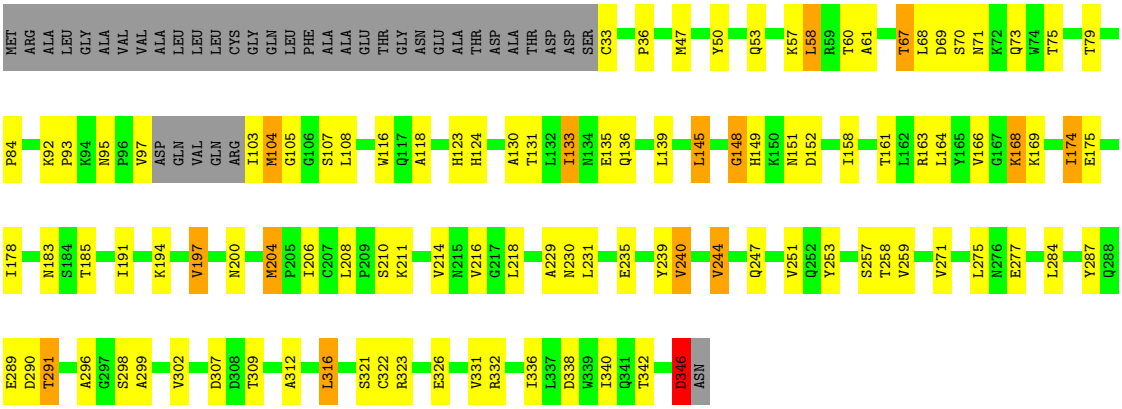
• Molecule 3: Haptoglobin

Chain F:



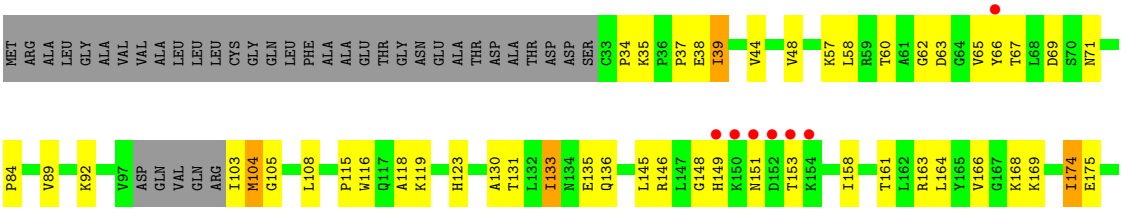
• Molecule 3: Haptoglobin

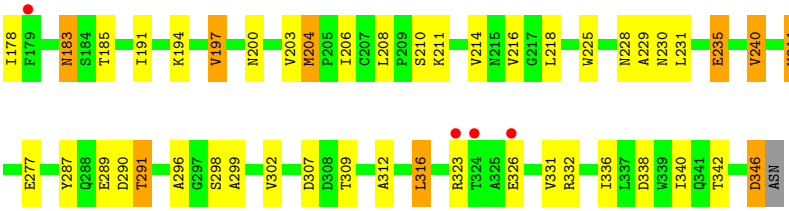
Chain I:



• Molecule 3: Haptoglobin

Chain L:





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

Chain M:

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

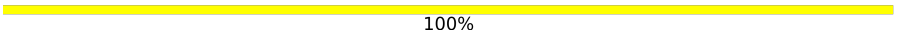
Chain O:

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

Chain Q:

• Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

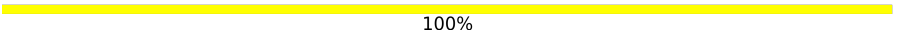


• Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

• Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.88Å 197.78Å 322.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 49.44 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.90) 99.0 (49.44-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.211 , 0.229 0.209 , 0.227	Depositor DCC
R_{free} test set	2251 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å^2)	75.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19196	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: HEM, FUC, OXY, NAG

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	0.59	0/1091	0.70	0/1480
1	D	0.61	0/1091	0.68	0/1480
1	G	0.56	0/1091	0.67	0/1480
1	J	0.35	0/1091	0.58	0/1480
2	B	0.57	0/1169	0.68	0/1580
2	E	0.48	0/1169	0.65	0/1580
2	H	0.63	0/1169	0.69	0/1580
2	K	0.44	0/1169	0.55	0/1580
3	C	0.57	0/2487	0.79	1/3377 (0.0%)
3	F	0.61	1/2487 (0.0%)	0.81	3/3377 (0.1%)
3	I	0.62	0/2487	0.81	3/3377 (0.1%)
3	L	0.51	0/2487	0.75	1/3377 (0.0%)
All	All	0.56	1/18988 (0.0%)	0.73	8/25748 (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
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	3
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	151	ASN	C-N	-5.51	1.21	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	346	ASP	CB-CG-OD2	5.56	123.30	118.30
3	F	322	CYS	CA-CB-SG	-5.23	104.59	114.00
3	I	136	GLN	N-CA-C	5.18	125.00	111.00
3	F	322	CYS	C-N-CA	-5.15	108.83	121.70
3	I	322	CYS	CA-CB-SG	-5.09	104.83	114.00
3	C	322	CYS	C-N-CA	-5.06	109.06	121.70
3	F	136	GLN	N-CA-C	5.04	124.61	111.00
3	L	136	GLN	N-CA-C	5.03	124.58	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	148	GLY	Peptide
3	C	257	SER	Peptide
3	F	148	GLY	Peptide
3	F	257	SER	Peptide
3	I	148	GLY	Peptide
3	I	257	SER	Peptide
3	L	148	GLY	Peptide
3	L	257	SER	Peptide
3	L	34	PRO	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	1064	0	1060	12	0
1	D	1064	0	1060	12	0
1	G	1064	0	1060	11	0
1	J	1064	0	1060	14	0
2	B	1144	0	1141	21	0
2	E	1144	0	1141	22	0
2	H	1144	0	1141	21	0
2	K	1144	0	1141	35	0
3	C	2428	0	2396	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2428	0	2394	54	0
3	I	2428	0	2395	57	0
3	L	2428	0	2397	66	0
4	M	28	0	25	1	0
4	O	28	0	25	1	0
4	Q	28	0	25	1	0
5	N	24	0	22	0	0
5	P	24	0	22	2	0
5	R	24	0	22	0	0
5	S	24	0	22	5	0
6	A	43	0	30	1	0
6	B	43	0	30	4	0
6	D	43	0	30	0	0
6	E	43	0	30	5	0
6	G	43	0	30	0	0
6	H	43	0	30	4	0
6	J	43	0	30	0	0
6	K	43	0	30	2	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	D	2	0	0	0	0
7	E	2	0	0	0	0
7	G	2	0	0	0	0
7	H	2	0	0	0	0
7	J	2	0	0	0	0
7	K	2	0	0	0	0
8	C	28	0	26	1	0
8	F	28	0	26	0	0
8	I	28	0	26	0	0
8	L	28	0	26	1	0
All	All	19196	0	18893	362	0

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 10.

All (362) 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:K:101[B]:GLU:HG3	3:L:230:ASN:HD22	1.12	1.12
2:E:101[B]:GLU:HG3	3:F:230:ASN:HD22	1.08	1.11
2:H:101[B]:GLU:HG3	3:I:230:ASN:HD22	1.10	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101[B]:GLU:HG3	3:C:230:ASN:HD22	1.12	1.07
3:F:92:LYS:H	3:F:204:MET:HE2	1.32	0.95
2:H:101[B]:GLU:HG3	3:I:230:ASN:ND2	1.86	0.91
3:F:118:ALA:HB3	3:F:130:ALA:HB3	1.54	0.89
2:E:101[B]:GLU:HG3	3:F:230:ASN:ND2	1.86	0.88
3:L:118:ALA:HB3	3:L:130:ALA:HB3	1.56	0.88
2:B:101[B]:GLU:HG3	3:C:230:ASN:ND2	1.90	0.88
3:C:118:ALA:HB3	3:C:130:ALA:HB3	1.56	0.87
2:H:22:GLU:OE1	2:H:117:ARG:NH2	2.09	0.86
3:L:235:GLU:HB2	5:S:2:FUC:H61	1.57	0.86
3:C:123:HIS:HB3	3:C:161:THR:HG23	1.61	0.83
3:I:118:ALA:HB3	3:I:130:ALA:HB3	1.61	0.82
3:I:60:THR:HG22	3:I:84:PRO:HB3	1.62	0.81
3:I:123:HIS:HB3	3:I:161:THR:HG23	1.62	0.81
3:L:123:HIS:HB3	3:L:161:THR:HG23	1.63	0.80
3:F:123:HIS:HB3	3:F:161:THR:HG23	1.62	0.80
1:G:122:HIS:HD2	2:H:30:ARG:HD3	1.48	0.78
3:C:60:THR:HG22	3:C:84:PRO:HB3	1.66	0.78
3:C:61:ALA:HB3	3:C:79:THR:HG22	1.66	0.77
1:J:122:HIS:HD2	2:K:30:ARG:HD3	1.49	0.77
1:A:122:HIS:HD2	2:B:30:ARG:HD3	1.50	0.77
2:K:101[B]:GLU:HG3	3:L:230:ASN:ND2	1.94	0.76
2:K:26:GLU:OE2	2:K:117:ARG:NH1	2.19	0.74
3:L:257:SER:HG	3:L:263:LYS:HZ3	1.35	0.73
3:I:61:ALA:HB3	3:I:79:THR:HG22	1.71	0.71
3:F:216:VAL:HA	3:F:244:VAL:HG22	1.73	0.70
3:F:151:ASN:OD1	3:F:152:ASP:N	2.25	0.70
3:L:216:VAL:HA	3:L:244:VAL:HG22	1.74	0.70
3:C:152:ASP:HB3	8:C:1003:NAG:H82	1.74	0.69
3:C:346:ASP:OD1	3:C:346:ASP:N	2.26	0.69
2:B:22:GLU:OE1	2:B:117:ARG:NH2	2.25	0.69
2:E:101[B]:GLU:CG	3:F:230:ASN:HD22	1.97	0.69
2:H:98:VAL:O	2:H:145:TYR:OH	2.07	0.68
3:I:346:ASP:OD1	3:I:346:ASP:N	2.27	0.68
3:C:216:VAL:HA	3:C:244:VAL:HG22	1.76	0.68
3:F:105:GLY:HA3	3:F:289:GLU:HG2	1.76	0.68
3:F:131:THR:HG21	3:F:299:ALA:N	2.08	0.68
2:B:98:VAL:O	2:B:145:TYR:OH	2.10	0.67
3:C:257:SER:HG	3:C:263:LYS:HZ3	1.40	0.67
3:C:158:ILE:O	3:C:161:THR:HB	1.95	0.67
3:F:346:ASP:OD1	3:F:346:ASP:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:HIS:HD2	2:E:30:ARG:HD3	1.60	0.66
3:L:158:ILE:O	3:L:161:THR:HB	1.95	0.66
3:L:346:ASP:N	3:L:346:ASP:OD1	2.29	0.66
3:I:158:ILE:O	3:I:161:THR:HB	1.96	0.66
2:H:101[B]:GLU:CG	3:I:230:ASN:HD22	1.98	0.65
3:C:174:ILE:HD12	3:C:191:ILE:HG23	1.79	0.65
3:F:131:THR:HG21	3:F:299:ALA:H	1.61	0.65
3:C:131:THR:HG21	3:C:299:ALA:N	2.11	0.65
2:E:22:GLU:OE1	2:E:117:ARG:NH2	2.30	0.65
3:I:216:VAL:HA	3:I:244:VAL:HG22	1.79	0.65
3:C:307:ASP:HB3	3:C:309:THR:HG23	1.78	0.64
3:I:131:THR:HG21	3:I:299:ALA:N	2.13	0.64
3:F:158:ILE:O	3:F:161:THR:HB	1.96	0.64
2:E:26:GLU:OE2	2:E:117:ARG:NH1	2.31	0.64
3:L:69:ASP:HB3	3:L:71:ASN:H	1.63	0.64
3:L:105:GLY:HA3	3:L:289:GLU:HG2	1.78	0.64
2:E:82:LYS:H	2:E:82:LYS:HD2	1.64	0.63
2:H:82:LYS:H	2:H:82:LYS:HD2	1.63	0.63
3:L:92:LYS:H	3:L:204:MET:HE2	1.63	0.63
2:B:82:LYS:H	2:B:82:LYS:HD2	1.64	0.62
2:B:101[B]:GLU:CG	3:C:230:ASN:HD22	2.01	0.62
3:C:105:GLY:HA3	3:C:289:GLU:HG2	1.82	0.62
6:K:201:HEM:HMC2	6:K:201:HEM:HBC2	1.82	0.62
1:J:94:ASP:OD1	1:J:96:VAL:HG22	2.00	0.61
3:C:34:PRO:HD2	3:F:68:LEU:HD21	1.82	0.61
3:L:307:ASP:HB3	3:L:309:THR:HG23	1.83	0.61
3:L:163:ARG:HG3	3:L:163:ARG:HH11	1.66	0.61
3:L:131:THR:HG21	3:L:299:ALA:N	2.16	0.60
3:F:174:ILE:HD12	3:F:191:ILE:HG23	1.83	0.60
3:L:104:MET:HE3	3:L:229:ALA:HA	1.81	0.60
3:I:105:GLY:HA3	3:I:289:GLU:HG2	1.84	0.60
3:I:174:ILE:HD12	3:I:191:ILE:HG23	1.83	0.60
3:I:307:ASP:HB3	3:I:309:THR:HG23	1.84	0.60
1:D:94:ASP:OD1	1:D:96:VAL:HG22	2.02	0.59
3:L:174:ILE:HD12	3:L:191:ILE:HG23	1.84	0.59
3:F:253:TYR:CE1	3:F:326:GLU:HG3	2.38	0.59
2:K:18:VAL:HG12	2:K:118:LEU:HD11	1.85	0.59
2:K:14:LEU:HD22	2:K:126:VAL:HG21	1.85	0.59
3:L:104:MET:HE2	3:L:323:ARG:HG3	1.85	0.59
3:F:69:ASP:HB3	3:F:71:ASN:H	1.68	0.59
3:C:69:ASP:HB3	3:C:71:ASN:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:94:ASP:OD1	1:G:96:VAL:HG22	2.02	0.58
3:C:296:ALA:HA	3:C:316:LEU:HB3	1.86	0.58
1:A:94:ASP:OD1	1:A:96:VAL:HG22	2.03	0.58
3:F:163:ARG:HG3	3:F:163:ARG:HH11	1.68	0.58
6:B:201:HEM:HMC2	6:B:201:HEM:HBC2	1.86	0.58
3:I:36:PRO:HG3	3:L:48:VAL:HG11	1.85	0.57
3:C:163:ARG:HG3	3:C:163:ARG:HH11	1.68	0.57
3:I:69:ASP:HB3	3:I:71:ASN:H	1.69	0.57
3:I:163:ARG:HG3	3:I:163:ARG:HH11	1.70	0.57
3:L:253:TYR:CE1	3:L:326:GLU:HG3	2.39	0.57
3:I:296:ALA:HA	3:I:316:LEU:HB3	1.86	0.57
6:E:201:HEM:HMC2	6:E:201:HEM:HBC2	1.88	0.56
3:F:124:HIS:CE1	3:F:148:GLY:HA2	2.40	0.56
1:J:123:ALA:HA	2:K:34:VAL:HG22	1.86	0.56
2:K:82:LYS:H	2:K:82:LYS:HD2	1.70	0.56
3:L:235:GLU:HB2	5:S:2:FUC:C6	2.32	0.56
3:F:307:ASP:HB3	3:F:309:THR:HG23	1.86	0.56
2:K:37:TRP:HA	3:L:287:TYR:HB3	1.88	0.55
2:B:26:GLU:OE2	2:B:117:ARG:NH1	2.39	0.55
2:B:93:CYS:HB2	2:B:145:TYR:CE1	2.41	0.55
3:C:47:MET:HG2	3:C:67:THR:HB	1.89	0.55
3:F:104:MET:HE3	3:F:229:ALA:HA	1.86	0.55
3:F:296:ALA:HA	3:F:316:LEU:HB3	1.89	0.55
6:H:201:HEM:HBC2	6:H:201:HEM:HMC2	1.88	0.55
3:I:131:THR:HG21	3:I:299:ALA:H	1.71	0.55
3:C:290:ASP:CG	3:C:291:THR:H	2.10	0.55
3:I:253:TYR:CE1	3:I:326:GLU:HG3	2.41	0.55
3:C:104:MET:HE3	3:C:229:ALA:HA	1.88	0.55
3:I:104:MET:HE3	3:I:229:ALA:HA	1.89	0.55
3:C:257:SER:OG	3:C:263:LYS:NZ	2.25	0.54
4:M:1:NAG:O3	4:M:2:NAG:N2	2.40	0.54
3:C:253:TYR:CE1	3:C:326:GLU:HG3	2.43	0.54
3:F:131:THR:HG23	3:F:298:SER:HA	1.89	0.54
3:I:131:THR:HG23	3:I:298:SER:HA	1.88	0.54
3:L:296:ALA:HA	3:L:316:LEU:HB3	1.90	0.53
2:B:37:TRP:HA	3:C:287:TYR:HB3	1.91	0.53
3:F:290:ASP:CG	3:F:291:THR:H	2.13	0.53
3:I:290:ASP:CG	3:I:291:THR:H	2.11	0.53
2:K:101[A]:GLU:HG3	2:K:102:ASN:N	2.24	0.52
3:C:131:THR:HG23	3:C:298:SER:HA	1.90	0.52
3:I:92:LYS:H	3:I:204:MET:HE2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:99:ASP:OD1	2:K:101[A]:GLU:HG2	2.09	0.52
1:A:1:VAL:H2	1:A:127:LYS:HD3	1.74	0.52
2:K:101[B]:GLU:HG2	3:L:228:ASN:CG	2.31	0.51
6:E:201:HEM:HBB2	6:E:201:HEM:HMB2	1.92	0.51
2:H:41:PHE:HB3	6:H:201:HEM:HMD2	1.92	0.51
6:H:201:HEM:HMB1	6:H:201:HEM:HBB2	1.93	0.51
3:C:92:LYS:H	3:C:204:MET:HE1	1.74	0.51
3:I:118:ALA:HB2	3:I:166:VAL:HG12	1.91	0.51
2:K:91:LEU:O	2:K:95:GLN:HB3	2.10	0.51
2:K:101[B]:GLU:HG2	3:L:228:ASN:OD1	2.11	0.51
2:K:101[B]:GLU:OE2	5:S:1:NAG:O7	2.29	0.51
1:A:1:VAL:N	1:A:127:LYS:HD3	2.26	0.50
3:C:131:THR:HG21	3:C:299:ALA:H	1.75	0.50
1:D:53:ASP:HA	1:D:56:LYS:HB3	1.93	0.50
3:L:183:ASN:CG	8:L:1002:NAG:O7	2.50	0.50
2:E:48:LEU:HD22	2:E:54:VAL:HG22	1.94	0.50
2:H:37:TRP:HA	3:I:287:TYR:HB3	1.93	0.50
2:H:93:CYS:HB2	2:H:145:TYR:CE1	2.47	0.50
3:L:290:ASP:CG	3:L:291:THR:H	2.13	0.50
3:I:47:MET:HG2	3:I:67:THR:HB	1.93	0.50
1:G:122:HIS:CD2	2:H:30:ARG:HD3	2.38	0.49
3:C:69:ASP:HB2	3:C:73:GLN:H	1.78	0.49
1:G:1:VAL:H1	1:G:127:LYS:HD3	1.77	0.49
2:H:26:GLU:OE2	2:H:117:ARG:NH1	2.44	0.49
1:G:93:VAL:HG22	1:G:98:PHE:CE2	2.47	0.49
6:B:201:HEM:HMB2	6:B:201:HEM:HBB2	1.93	0.49
2:B:48:LEU:HD22	2:B:54:VAL:HG22	1.94	0.49
1:A:122:HIS:CD2	2:B:30:ARG:HD3	2.40	0.48
3:C:118:ALA:HB2	3:C:166:VAL:HG12	1.95	0.48
1:J:53:ASP:HA	1:J:56:LYS:HB3	1.95	0.48
2:E:93:CYS:HB2	2:E:145:TYR:CE1	2.48	0.48
3:I:104:MET:HE2	3:I:323:ARG:HG3	1.95	0.48
1:J:122:HIS:CD2	2:K:30:ARG:HD3	2.39	0.48
2:B:41:PHE:HB3	6:B:201:HEM:HMD2	1.95	0.48
2:H:122:PHE:CE2	2:H:127:GLN:HB2	2.48	0.48
1:D:93:VAL:HG22	1:D:98:PHE:CE2	2.49	0.48
2:H:48:LEU:HD22	2:H:54:VAL:HG22	1.96	0.48
2:K:109:VAL:O	2:K:113:VAL:HG13	2.13	0.48
3:C:92:LYS:NZ	3:C:309:THR:HG22	2.28	0.48
3:C:107:SER:HB2	3:C:239:TYR:O	2.14	0.48
2:E:66:LYS:HE3	6:E:201:HEM:HAA1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:149:HIS:NE2	3:F:161:THR:HG21	2.29	0.48
2:K:8:LYS:O	2:K:12:LEU:HB2	2.14	0.48
2:E:122:PHE:CE2	2:E:127:GLN:HB2	2.49	0.47
3:I:69:ASP:HB2	3:I:73:GLN:H	1.79	0.47
3:L:131:THR:HG23	3:L:298:SER:HA	1.95	0.47
3:F:235:GLU:HB2	5:P:2:FUC:H61	1.96	0.47
3:L:135:GLU:O	3:L:197:VAL:HG23	2.14	0.47
3:C:60:THR:CG2	3:C:84:PRO:HB3	2.42	0.47
2:H:66:LYS:HE3	6:H:201:HEM:HAA1	1.97	0.47
3:I:103:ILE:HD13	3:I:240:VAL:HG22	1.96	0.47
2:B:79:ASP:OD1	2:B:79:ASP:N	2.46	0.47
3:I:92:LYS:H	3:I:204:MET:CE	2.27	0.47
1:J:1:VAL:N	1:J:127:LYS:HD3	2.30	0.47
1:G:42:TYR:CE2	1:G:93:VAL:HA	2.50	0.47
1:A:93:VAL:HG22	1:A:98:PHE:CE2	2.49	0.47
2:B:66:LYS:HE3	6:B:201:HEM:HAA1	1.96	0.47
3:F:235:GLU:HA	5:P:2:FUC:H61	1.97	0.47
3:F:336:ILE:HD12	3:F:340:ILE:HD11	1.97	0.47
1:J:31:ARG:HD3	2:K:127:GLN:OE1	2.14	0.47
2:E:41:PHE:HB3	6:E:201:HEM:HMD2	1.96	0.47
3:F:116:TRP:O	3:F:131:THR:HA	2.15	0.47
2:B:14:LEU:HD21	2:B:118:LEU:HD23	1.96	0.47
1:J:93:VAL:HG22	1:J:98:PHE:CE2	2.50	0.47
3:F:69:ASP:HB2	3:F:73:GLN:H	1.80	0.46
3:L:69:ASP:HB3	3:L:71:ASN:N	2.29	0.46
3:C:93:PRO:HG3	3:C:116:TRP:CZ3	2.51	0.46
3:I:336:ILE:HD12	3:I:340:ILE:HD11	1.97	0.46
2:K:142:ALA:O	2:K:145:TYR:HB2	2.15	0.46
3:F:135:GLU:O	3:F:197:VAL:HG23	2.16	0.46
2:K:14:LEU:O	2:K:18:VAL:HG13	2.15	0.46
3:L:131:THR:HG21	3:L:299:ALA:H	1.80	0.46
3:L:118:ALA:HB2	3:L:166:VAL:HG12	1.97	0.46
3:C:135:GLU:O	3:C:197:VAL:HG23	2.16	0.46
3:F:104:MET:HE2	3:F:323:ARG:HG3	1.96	0.46
3:I:206:ILE:HG21	3:I:312:ALA:HB2	1.97	0.46
3:F:133:ILE:CG1	3:F:208:LEU:HD21	2.46	0.46
1:J:138:SER:HB2	3:L:271:VAL:HG13	1.98	0.46
1:J:107:VAL:HG13	2:K:115:ALA:HB2	1.98	0.46
2:E:67:VAL:O	2:E:70:SER:HB3	2.16	0.46
3:L:175:GLU:HB2	3:L:194:LYS:HA	1.98	0.46
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:14:LEU:HD21	2:H:118:LEU:HD23	1.97	0.46
3:I:57:LYS:HB2	3:I:57:LYS:HE3	1.66	0.46
3:L:103:ILE:HD13	3:L:240:VAL:HG22	1.97	0.46
3:I:92:LYS:NZ	3:I:309:THR:HG22	2.31	0.45
3:C:257:SER:HG	3:C:258:THR:HA	1.80	0.45
2:H:79:ASP:OD1	2:H:79:ASP:N	2.49	0.45
6:K:201:HEM:HMB2	6:K:201:HEM:HBB2	1.98	0.45
3:I:284:LEU:HD22	3:I:290:ASP:HB2	1.97	0.45
2:K:40:ARG:HH22	3:L:289:GLU:CD	2.19	0.45
4:Q:1:NAG:O3	4:Q:2:NAG:N2	2.50	0.45
3:L:89:VAL:O	3:L:204:MET:HE3	2.17	0.45
3:L:163:ARG:HG3	3:L:163:ARG:NH1	2.30	0.45
3:I:135:GLU:O	3:I:197:VAL:HG23	2.16	0.45
2:K:131:GLN:HA	2:K:134:VAL:HG22	1.97	0.45
2:B:122:PHE:CE2	2:B:127:GLN:HB2	2.51	0.45
3:F:145:LEU:HD12	3:F:145:LEU:HA	1.86	0.45
3:I:92:LYS:HB2	3:I:204:MET:HE1	1.97	0.45
3:C:48:VAL:HG11	3:F:36:PRO:HG3	1.99	0.45
3:C:57:LYS:HB2	3:C:57:LYS:HE3	1.63	0.45
3:C:337:LEU:HD23	3:C:337:LEU:HA	1.81	0.45
4:O:1:NAG:O3	4:O:2:NAG:N2	2.49	0.45
3:C:58:LEU:HD23	3:C:58:LEU:HA	1.85	0.45
1:G:53:ASP:HA	1:G:56:LYS:HB3	1.98	0.45
1:A:42:TYR:CE2	1:A:93:VAL:HA	2.52	0.45
1:G:1:VAL:N	1:G:127:LYS:HD3	2.30	0.45
2:B:18:VAL:CG1	2:B:118:LEU:HD21	2.47	0.44
3:C:206:ILE:HG21	3:C:312:ALA:HB2	2.00	0.44
2:E:98:VAL:O	2:E:145:TYR:OH	2.20	0.44
2:K:28:LEU:O	2:K:32:LEU:HD13	2.17	0.44
3:F:118:ALA:HB2	3:F:166:VAL:HG12	2.00	0.44
3:L:92:LYS:H	3:L:204:MET:CE	2.27	0.44
3:C:197:VAL:HG11	3:C:203:VAL:HG11	1.98	0.44
2:H:57:ASN:HA	2:H:58:PRO:HD3	1.90	0.44
2:K:71:PHE:CZ	2:K:137:VAL:HG21	2.53	0.44
2:K:127:GLN:O	2:K:131:GLN:HG2	2.17	0.44
3:L:336:ILE:HD12	3:L:340:ILE:HD11	2.00	0.44
3:C:269:VAL:HG23	3:C:271:VAL:H	1.82	0.44
3:L:115:PRO:HB2	3:L:204:MET:HG2	2.00	0.44
3:F:163:ARG:HG3	3:F:163:ARG:NH1	2.32	0.44
3:F:290:ASP:OD2	3:F:321:SER:HB2	2.18	0.44
2:K:81:LEU:HD12	2:K:81:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:LYS:CE	3:C:309:THR:HG22	2.47	0.44
3:F:175:GLU:HB2	3:F:194:LYS:HA	1.99	0.44
3:F:206:ILE:HG21	3:F:312:ALA:HB2	2.00	0.44
3:I:107:SER:HB2	3:I:239:TYR:O	2.17	0.44
3:L:63:ASP:OD2	3:L:65:VAL:HB	2.17	0.44
1:D:1:VAL:N	1:D:127:LYS:HD3	2.33	0.44
2:K:144:LYS:HD3	2:K:144:LYS:HA	1.81	0.44
3:C:163:ARG:HG3	3:C:163:ARG:NH1	2.32	0.44
3:I:175:GLU:HB2	3:I:194:LYS:HA	1.99	0.44
1:A:66:LEU:O	1:A:70:VAL:HG23	2.17	0.43
2:E:19:ASN:O	2:E:23:VAL:HG13	2.18	0.43
2:E:81:LEU:HD12	2:E:81:LEU:HA	1.88	0.43
1:G:2:LEU:HD12	1:G:2:LEU:HA	1.81	0.43
1:G:38:THR:O	1:G:41:THR:HB	2.18	0.43
3:C:145:LEU:HD12	3:C:145:LEU:HA	1.90	0.43
3:F:337:LEU:HD23	3:F:337:LEU:HA	1.83	0.43
1:J:66:LEU:O	1:J:70:VAL:HG23	2.17	0.43
3:L:116:TRP:O	3:L:131:THR:HA	2.17	0.43
3:F:197:VAL:HG11	3:F:203:VAL:HG11	2.00	0.43
2:B:18:VAL:HG12	2:B:118:LEU:HD21	2.00	0.43
1:A:53:ASP:HA	1:A:56:LYS:HB3	2.01	0.43
1:J:42:TYR:CE2	1:J:93:VAL:HA	2.53	0.43
3:C:284:LEU:HD22	3:C:290:ASP:HB2	2.01	0.43
2:E:18:VAL:HG12	2:E:118:LEU:HD21	2.01	0.43
3:L:257:SER:HG	3:L:263:LYS:NZ	2.09	0.43
1:A:38:THR:O	1:A:41:THR:HB	2.19	0.43
3:C:175:GLU:HB2	3:C:194:LYS:HA	1.99	0.43
1:G:76:LEU:HA	1:G:76:LEU:HD23	1.76	0.43
3:I:194:LYS:HE3	3:I:194:LYS:HB2	1.79	0.43
3:C:137:TRP:CZ2	3:C:192:LYS:HD2	2.54	0.43
3:I:58:LEU:HD23	3:I:58:LEU:HA	1.86	0.43
1:J:76:LEU:HD23	1:J:76:LEU:HA	1.73	0.42
3:F:194:LYS:HE3	3:F:194:LYS:HB2	1.84	0.42
3:L:257:SER:HG	3:L:258:THR:HA	1.84	0.42
3:C:103:ILE:HD13	3:C:240:VAL:HG22	2.01	0.42
3:C:116:TRP:O	3:C:131:THR:HA	2.19	0.42
3:C:336:ILE:HD12	3:C:340:ILE:HD11	2.02	0.42
3:F:256:GLY:HA3	3:F:257:SER:HA	1.94	0.42
2:K:101[B]:GLU:HG2	3:L:228:ASN:ND2	2.34	0.42
2:B:24:GLY:HA2	2:B:68:LEU:HD23	2.02	0.42
3:I:149:HIS:NE2	3:I:161:THR:HG21	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:269:VAL:HG23	3:F:271:VAL:H	1.83	0.42
2:H:18:VAL:CG1	2:H:118:LEU:HD21	2.50	0.42
3:L:133:ILE:CG1	3:L:208:LEU:HD21	2.50	0.42
3:L:119:LYS:HB2	3:L:225:TRP:CD1	2.54	0.42
3:L:269:VAL:HG23	3:L:271:VAL:H	1.83	0.42
3:I:251:VAL:HG22	3:I:275:LEU:HD13	2.02	0.42
6:A:201:HEM:CMB	6:A:201:HEM:HBB2	2.50	0.42
1:D:28:ALA:CB	1:D:105:LEU:HD13	2.50	0.42
3:L:307:ASP:O	3:L:309:THR:HG23	2.20	0.42
1:D:2:LEU:HA	1:D:2:LEU:HD12	1.82	0.42
3:I:163:ARG:HG3	3:I:163:ARG:NH1	2.33	0.42
3:C:256:GLY:HA3	3:C:257:SER:HA	1.95	0.42
3:C:257:SER:HG	3:C:263:LYS:NZ	2.10	0.42
3:F:257:SER:OG	3:F:258:THR:HA	2.20	0.42
3:I:130:ALA:O	3:I:139:LEU:O	2.37	0.42
3:I:50:TYR:OH	3:L:37:PRO:HG2	2.20	0.41
3:I:151:ASN:OD1	3:I:152:ASP:N	2.53	0.41
2:K:83:GLY:HA2	2:K:86:ALA:HB2	2.02	0.41
3:C:92:LYS:HB2	3:C:204:MET:HE1	2.02	0.41
1:D:28:ALA:HB2	1:D:105:LEU:HD13	2.03	0.41
1:D:66:LEU:O	1:D:70:VAL:HG23	2.20	0.41
3:F:60:THR:HG23	3:F:62:GLY:O	2.20	0.41
3:F:168:LYS:O	3:F:170:GLN:N	2.53	0.41
3:F:267:SER:HA	3:F:268:PRO:HD2	1.86	0.41
3:I:145:LEU:HD12	3:I:145:LEU:HA	1.80	0.41
3:L:235:GLU:HA	5:S:2:FUC:H63	2.03	0.41
1:D:99:LYS:HD3	3:F:229:ALA:O	2.20	0.41
3:L:146:ARG:HD3	3:L:151:ASN:HA	2.03	0.41
2:H:40:ARG:HH22	3:I:289:GLU:CD	2.23	0.41
3:I:133:ILE:CG1	3:I:208:LEU:HD21	2.50	0.41
3:L:58:LEU:HD22	3:L:84:PRO:HB2	2.03	0.41
3:L:249:LYS:HB3	3:L:249:LYS:HE2	1.90	0.41
1:A:76:LEU:HA	1:A:76:LEU:HD23	1.73	0.41
2:E:100:PRO:HA	2:E:103:PHE:CD2	2.56	0.41
3:I:124:HIS:CE1	3:I:148:GLY:HA2	2.55	0.41
3:L:66:TYR:CZ	3:L:84:PRO:HD3	2.55	0.41
2:B:40:ARG:HH22	3:C:289:GLU:CD	2.24	0.41
2:K:19:ASN:O	2:K:23:VAL:HG13	2.20	0.41
3:L:235:GLU:CB	5:S:2:FUC:H61	2.38	0.41
1:A:52:SER:HB3	1:A:55:VAL:HG13	2.02	0.41
2:E:88:LEU:HD11	6:E:201:HEM:HMA1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:VAL:HG12	2:H:118:LEU:HD21	2.02	0.41
1:J:38:THR:O	1:J:41:THR:HB	2.21	0.41
2:K:15:TRP:O	2:K:18:VAL:HG22	2.21	0.41
3:L:149:HIS:HB3	3:L:153:THR:OG1	2.21	0.41
3:C:104:MET:HE2	3:C:323:ARG:HG3	2.02	0.41
3:C:147:LEU:HD23	3:C:147:LEU:HA	1.91	0.41
3:C:251:VAL:HG22	3:C:275:LEU:HD13	2.02	0.41
1:D:42:TYR:CE2	1:D:93:VAL:HA	2.56	0.41
2:E:18:VAL:CG1	2:E:118:LEU:HD21	2.50	0.41
3:I:93:PRO:HG3	3:I:116:TRP:CZ3	2.56	0.41
2:K:26:GLU:OE1	2:K:30:ARG:NH2	2.42	0.41
2:E:14:LEU:HD21	2:E:118:LEU:HD23	2.04	0.40
3:L:194:LYS:HB2	3:L:194:LYS:HE3	1.82	0.40
3:L:206:ILE:HD13	3:L:312:ALA:HB2	2.03	0.40
3:F:151:ASN:OD1	3:F:152:ASP:OD1	2.40	0.40
3:F:260:PRO:HA	3:F:263:LYS:HE2	2.03	0.40
3:L:39:ILE:HG21	3:L:39:ILE:HD13	1.69	0.40
3:C:124:HIS:CE1	3:C:148:GLY:HA2	2.57	0.40
3:I:60:THR:CG2	3:I:84:PRO:HB3	2.40	0.40
3:I:92:LYS:CE	3:I:309:THR:HG22	2.51	0.40
3:I:104:MET:CE	3:I:323:ARG:HG3	2.51	0.40
3:L:58:LEU:HD23	3:L:58:LEU:HA	1.80	0.40
3:F:92:LYS:N	3:F:204:MET:HE2	2.16	0.40
3:I:206:ILE:HD13	3:I:312:ALA:HB2	2.02	0.40
3:L:60:THR:HG23	3:L:62:GLY:O	2.22	0.40
3:L:197:VAL:HG11	3:L:203:VAL:HG11	2.02	0.40
3:L:259:VAL:HG11	3:L:262:LYS:HD2	2.03	0.40
2:E:24:GLY:HA2	2:E:68:LEU:HD23	2.03	0.40
3:F:66:TYR:CZ	3:F:84:PRO:HD3	2.57	0.40
2:K:18:VAL:CG1	2:K:118:LEU:HD21	2.51	0.40
3:L:66:TYR:CE1	3:L:84:PRO:HD3	2.56	0.40

There are no symmetry-related clashes.

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	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
1	D	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
1	G	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
1	J	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
2	B	145/146 (99%)	143 (99%)	2 (1%)	0	100	100
2	E	145/146 (99%)	142 (98%)	3 (2%)	0	100	100
2	H	145/146 (99%)	143 (99%)	2 (1%)	0	100	100
2	K	145/146 (99%)	142 (98%)	3 (2%)	0	100	100
3	C	305/347 (88%)	288 (94%)	15 (5%)	2 (1%)	22	54
3	F	305/347 (88%)	284 (93%)	20 (7%)	1 (0%)	41	71
3	I	305/347 (88%)	287 (94%)	15 (5%)	3 (1%)	15	45
3	L	305/347 (88%)	285 (93%)	18 (6%)	2 (1%)	22	54
All	All	2356/2536 (93%)	2250 (96%)	98 (4%)	8 (0%)	41	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	258	THR
3	L	169	LYS
3	L	258	THR
3	C	169	LYS
3	C	258	THR
3	I	168	LYS
3	I	169	LYS
3	I	258	THR

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	111/111 (100%)	97 (87%)	14 (13%)	4 13
1	D	111/111 (100%)	97 (87%)	14 (13%)	4 13
1	G	111/111 (100%)	97 (87%)	14 (13%)	4 13
1	J	111/111 (100%)	97 (87%)	14 (13%)	4 13
2	B	120/119 (101%)	101 (84%)	19 (16%)	2 8
2	E	120/119 (101%)	102 (85%)	18 (15%)	3 9
2	H	120/119 (101%)	103 (86%)	17 (14%)	3 10
2	K	120/119 (101%)	100 (83%)	20 (17%)	2 6
3	C	268/296 (90%)	225 (84%)	43 (16%)	2 7
3	F	268/296 (90%)	230 (86%)	38 (14%)	3 10
3	I	268/296 (90%)	225 (84%)	43 (16%)	2 7
3	L	268/296 (90%)	229 (85%)	39 (15%)	3 9
All	All	1996/2104 (95%)	1703 (85%)	293 (15%)	3 9

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	16	LYS
1	A	38	THR
1	A	41	THR
1	A	55	VAL
1	A	80	LEU
1	A	84	SER
1	A	86	LEU
1	A	93	VAL
1	A	105	LEU
1	A	106	LEU
1	A	109	LEU
1	A	122	HIS
1	A	129	LEU
2	B	4	SER
2	B	8	LYS
2	B	12	LEU
2	B	18	VAL
2	B	43	GLU
2	B	67	VAL
2	B	68	LEU
2	B	71	PHE

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Mol	Chain	Res	Type
2	B	75	LEU
2	B	78	LEU
2	B	81	LEU
2	B	82	LYS
2	B	91	LEU
2	B	113	VAL
2	B	118	LEU
2	B	126	VAL
2	B	127	GLN
2	B	137	VAL
2	B	144	LYS
3	C	53	GLN
3	C	58	LEU
3	C	60	THR
3	C	67	THR
3	C	68	LEU
3	C	70	SER
3	C	75	THR
3	C	82	LYS
3	C	90	CYS
3	C	95	ASN
3	C	97	VAL
3	C	104	MET
3	C	108	LEU
3	C	133	ILE
3	C	145	LEU
3	C	164	LEU
3	C	168	LYS
3	C	174	ILE
3	C	178	ILE
3	C	183	ASN
3	C	185	THR
3	C	197	VAL
3	C	200	ASN
3	C	204	MET
3	C	210	SER
3	C	214	VAL
3	C	218	LEU
3	C	231	LEU
3	C	235	GLU
3	C	240	VAL
3	C	244	VAL

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Mol	Chain	Res	Type
3	C	247	GLN
3	C	259	VAL
3	C	277	GLU
3	C	291	THR
3	C	302	VAL
3	C	316	LEU
3	C	321	SER
3	C	331	VAL
3	C	332	ARG
3	C	338	ASP
3	C	342	THR
3	C	346	ASP
1	D	2	LEU
1	D	16	LYS
1	D	38	THR
1	D	41	THR
1	D	55	VAL
1	D	80	LEU
1	D	84	SER
1	D	86	LEU
1	D	93	VAL
1	D	105	LEU
1	D	106	LEU
1	D	109	LEU
1	D	122	HIS
1	D	129	LEU
2	E	4	SER
2	E	8	LYS
2	E	12	LEU
2	E	23	VAL
2	E	43	GLU
2	E	67	VAL
2	E	71	PHE
2	E	75	LEU
2	E	78	LEU
2	E	81	LEU
2	E	82	LYS
2	E	91	LEU
2	E	113	VAL
2	E	118	LEU
2	E	126	VAL
2	E	127	GLN

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Mol	Chain	Res	Type
2	E	137	VAL
2	E	144	LYS
3	F	38	GLU
3	F	39	ILE
3	F	44	VAL
3	F	57	LYS
3	F	67	THR
3	F	69	ASP
3	F	104	MET
3	F	108	LEU
3	F	133	ILE
3	F	145	LEU
3	F	164	LEU
3	F	168	LYS
3	F	174	ILE
3	F	178	ILE
3	F	183	ASN
3	F	185	THR
3	F	197	VAL
3	F	200	ASN
3	F	204	MET
3	F	210	SER
3	F	211	LYS
3	F	214	VAL
3	F	218	LEU
3	F	231	LEU
3	F	235	GLU
3	F	240	VAL
3	F	247	GLN
3	F	259	VAL
3	F	277	GLU
3	F	291	THR
3	F	302	VAL
3	F	316	LEU
3	F	321	SER
3	F	331	VAL
3	F	332	ARG
3	F	338	ASP
3	F	342	THR
3	F	346	ASP
1	G	2	LEU
1	G	16	LYS

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Mol	Chain	Res	Type
1	G	38	THR
1	G	41	THR
1	G	55	VAL
1	G	80	LEU
1	G	84	SER
1	G	86	LEU
1	G	93	VAL
1	G	105	LEU
1	G	106	LEU
1	G	109	LEU
1	G	122	HIS
1	G	129	LEU
2	H	4	SER
2	H	8	LYS
2	H	12	LEU
2	H	18	VAL
2	H	43	GLU
2	H	67	VAL
2	H	71	PHE
2	H	75	LEU
2	H	78	LEU
2	H	81	LEU
2	H	82	LYS
2	H	91	LEU
2	H	118	LEU
2	H	126	VAL
2	H	127	GLN
2	H	137	VAL
2	H	144	LYS
3	I	33	CYS
3	I	53	GLN
3	I	58	LEU
3	I	67	THR
3	I	68	LEU
3	I	70	SER
3	I	75	THR
3	I	95	ASN
3	I	97	VAL
3	I	104	MET
3	I	108	LEU
3	I	133	ILE
3	I	145	LEU

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Mol	Chain	Res	Type
3	I	164	LEU
3	I	168	LYS
3	I	174	ILE
3	I	178	ILE
3	I	183	ASN
3	I	185	THR
3	I	197	VAL
3	I	200	ASN
3	I	204	MET
3	I	210	SER
3	I	211	LYS
3	I	214	VAL
3	I	218	LEU
3	I	231	LEU
3	I	235	GLU
3	I	240	VAL
3	I	244	VAL
3	I	247	GLN
3	I	259	VAL
3	I	271	VAL
3	I	277	GLU
3	I	291	THR
3	I	302	VAL
3	I	316	LEU
3	I	321	SER
3	I	331	VAL
3	I	332	ARG
3	I	338	ASP
3	I	342	THR
3	I	346	ASP
1	J	2	LEU
1	J	16	LYS
1	J	38	THR
1	J	41	THR
1	J	55	VAL
1	J	80	LEU
1	J	84	SER
1	J	86	LEU
1	J	93	VAL
1	J	105	LEU
1	J	106	LEU
1	J	109	LEU

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Mol	Chain	Res	Type
1	J	122	HIS
1	J	129	LEU
2	K	4	SER
2	K	12	LEU
2	K	23	VAL
2	K	43	GLU
2	K	61	LYS
2	K	67	VAL
2	K	68	LEU
2	K	71	PHE
2	K	75	LEU
2	K	78	LEU
2	K	81	LEU
2	K	91	LEU
2	K	104	ARG
2	K	112	VAL
2	K	118	LEU
2	K	126	VAL
2	K	127	GLN
2	K	137	VAL
2	K	144	LYS
2	K	145	TYR
3	L	35	LYS
3	L	38	GLU
3	L	39	ILE
3	L	44	VAL
3	L	57	LYS
3	L	67	THR
3	L	104	MET
3	L	108	LEU
3	L	133	ILE
3	L	145	LEU
3	L	164	LEU
3	L	168	LYS
3	L	174	ILE
3	L	178	ILE
3	L	183	ASN
3	L	185	THR
3	L	197	VAL
3	L	200	ASN
3	L	204	MET
3	L	210	SER

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Mol	Chain	Res	Type
3	L	211	LYS
3	L	214	VAL
3	L	218	LEU
3	L	231	LEU
3	L	235	GLU
3	L	240	VAL
3	L	244	VAL
3	L	247	GLN
3	L	259	VAL
3	L	271	VAL
3	L	277	GLU
3	L	291	THR
3	L	302	VAL
3	L	316	LEU
3	L	331	VAL
3	L	332	ARG
3	L	338	ASP
3	L	342	THR
3	L	346	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
3	C	230	ASN
1	D	122	HIS
3	F	230	ASN
1	G	122	HIS
3	I	230	ASN
1	J	122	HIS
3	L	230	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

14 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	$\#\|Z\| > 2$
4	NAG	M	1	3,4	14,14,15	2.42	6 (42%)	17,19,21	3.15	10 (58%)
4	NAG	M	2	4	14,14,15	2.44	7 (50%)	17,19,21	1.63	3 (17%)
5	NAG	N	1	5,3	14,14,15	2.11	5 (35%)	17,19,21	2.35	6 (35%)
5	FUC	N	2	5	10,10,11	2.70	4 (40%)	14,14,16	2.60	4 (28%)
4	NAG	O	1	3,4	14,14,15	2.50	6 (42%)	17,19,21	3.64	13 (76%)
4	NAG	O	2	4	14,14,15	2.10	6 (42%)	17,19,21	1.49	3 (17%)
5	NAG	P	1	5,3	14,14,15	2.06	6 (42%)	17,19,21	2.30	6 (35%)
5	FUC	P	2	5	10,10,11	2.41	5 (50%)	14,14,16	2.27	4 (28%)
4	NAG	Q	1	3,4	14,14,15	2.19	6 (42%)	17,19,21	3.46	9 (52%)
4	NAG	Q	2	4	14,14,15	2.30	7 (50%)	17,19,21	1.60	2 (11%)
5	NAG	R	1	5,3	14,14,15	2.08	5 (35%)	17,19,21	2.14	5 (29%)
5	FUC	R	2	5	10,10,11	2.73	5 (50%)	14,14,16	2.86	5 (35%)
5	NAG	S	1	5,3	14,14,15	0.41	0	17,19,21	1.40	2 (11%)
5	FUC	S	2	5	10,10,11	0.47	0	14,14,16	0.96	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	M	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
5	NAG	N	1	5,3	-	0/6/23/26	0/1/1/1
5	FUC	N	2	5	-	-	0/1/1/1
4	NAG	O	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
5	NAG	P	1	5,3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUC	P	2	5	-	-	0/1/1/1
4	NAG	Q	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
5	NAG	R	1	5,3	-	1/6/23/26	0/1/1/1
5	FUC	R	2	5	-	-	0/1/1/1
5	NAG	S	1	5,3	-	0/6/23/26	0/1/1/1
5	FUC	S	2	5	-	-	0/1/1/1

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	2	FUC	O5-C5	5.83	1.56	1.43
5	N	2	FUC	O5-C5	5.68	1.55	1.43
4	O	1	NAG	C2-N2	4.87	1.54	1.46
5	N	1	NAG	O5-C5	4.68	1.52	1.43
4	O	1	NAG	C7-N2	4.67	1.50	1.34
5	R	1	NAG	O5-C5	4.58	1.52	1.43
5	P	2	FUC	O5-C5	4.53	1.53	1.43
4	M	2	NAG	O5-C5	4.51	1.52	1.43
4	M	1	NAG	C2-N2	4.41	1.53	1.46
4	Q	2	NAG	O5-C5	4.41	1.52	1.43
4	M	1	NAG	C7-N2	4.30	1.49	1.34
5	R	2	FUC	C2-C3	-4.25	1.46	1.52
4	Q	1	NAG	C7-N2	4.18	1.48	1.34
5	N	2	FUC	C2-C3	-4.07	1.46	1.52
4	M	2	NAG	C2-N2	3.94	1.53	1.46
4	O	2	NAG	O5-C5	3.77	1.51	1.43
5	P	1	NAG	O5-C5	3.71	1.51	1.43
5	P	1	NAG	C7-N2	3.63	1.46	1.34
4	Q	1	NAG	C2-N2	3.60	1.52	1.46
5	N	1	NAG	C7-N2	3.55	1.46	1.34
5	R	1	NAG	C7-N2	3.55	1.46	1.34
4	M	2	NAG	C7-N2	3.48	1.46	1.34
5	N	2	FUC	C4-C3	-3.34	1.43	1.52
4	Q	2	NAG	C7-N2	3.33	1.45	1.34
4	M	2	NAG	C4-C3	-3.28	1.44	1.52
4	O	2	NAG	C7-N2	3.23	1.45	1.34
5	R	1	NAG	O4-C4	3.19	1.50	1.43
5	P	2	FUC	O3-C3	3.06	1.50	1.43
4	Q	2	NAG	C2-N2	3.06	1.51	1.46
4	Q	1	NAG	O4-C4	3.03	1.50	1.43
4	O	2	NAG	C4-C3	-3.03	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	2	FUC	C4-C3	-3.00	1.44	1.52
4	O	1	NAG	O5-C5	2.97	1.49	1.43
4	M	1	NAG	O4-C4	2.96	1.50	1.43
5	N	1	NAG	O4-C4	2.94	1.49	1.43
4	Q	2	NAG	C4-C3	-2.93	1.44	1.52
5	P	2	FUC	C2-C3	-2.83	1.48	1.52
4	M	1	NAG	O5-C5	2.82	1.49	1.43
5	R	2	FUC	C4-C3	-2.81	1.45	1.52
4	M	2	NAG	C1-C2	2.80	1.56	1.52
5	P	1	NAG	C2-N2	2.76	1.51	1.46
5	P	1	NAG	C4-C3	-2.75	1.45	1.52
4	Q	1	NAG	O5-C5	2.74	1.49	1.43
4	M	1	NAG	O5-C1	-2.73	1.39	1.43
4	M	2	NAG	O3-C3	2.66	1.49	1.43
4	Q	2	NAG	C1-C2	2.59	1.56	1.52
4	M	1	NAG	C3-C2	-2.56	1.47	1.52
4	O	2	NAG	C2-N2	2.55	1.50	1.46
4	O	2	NAG	O3-C3	2.52	1.48	1.43
4	O	1	NAG	O5-C1	-2.52	1.39	1.43
5	P	2	FUC	O5-C1	-2.51	1.39	1.43
4	O	1	NAG	O4-C4	2.49	1.48	1.43
4	Q	2	NAG	O4-C4	2.46	1.48	1.43
5	P	1	NAG	O3-C3	2.46	1.48	1.43
5	N	1	NAG	C4-C3	-2.43	1.46	1.52
4	Q	2	NAG	O3-C3	2.40	1.48	1.43
4	O	1	NAG	C3-C2	-2.37	1.47	1.52
4	Q	1	NAG	O5-C1	-2.36	1.39	1.43
4	O	2	NAG	O4-C4	2.32	1.48	1.43
5	R	2	FUC	O3-C3	2.27	1.48	1.43
5	P	1	NAG	O4-C4	2.27	1.48	1.43
5	R	2	FUC	O4-C4	2.25	1.48	1.43
5	N	2	FUC	O4-C4	2.24	1.48	1.43
4	Q	1	NAG	O3-C3	2.24	1.48	1.43
4	M	2	NAG	O4-C4	2.20	1.48	1.43
5	R	1	NAG	C4-C3	-2.18	1.46	1.52
5	R	1	NAG	O3-C3	2.10	1.47	1.43
5	N	1	NAG	C2-N2	2.10	1.49	1.46

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	1	NAG	O5-C1-C2	8.53	124.76	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	1	NAG	O5-C1-C2	8.04	123.98	111.29
5	R	2	FUC	O5-C5-C6	6.71	121.78	107.33
5	N	2	FUC	O5-C5-C6	6.37	121.05	107.33
4	M	1	NAG	O5-C1-C2	6.12	120.95	111.29
4	O	1	NAG	C2-N2-C7	6.05	131.52	122.90
5	P	1	NAG	C2-N2-C7	-5.98	114.39	122.90
5	N	1	NAG	C2-N2-C7	-5.71	114.77	122.90
5	R	2	FUC	C1-O5-C5	-5.53	100.24	112.78
5	R	1	NAG	C2-N2-C7	-5.35	115.29	122.90
4	M	2	NAG	C2-N2-C7	-5.11	115.62	122.90
5	N	2	FUC	C1-O5-C5	-5.09	101.24	112.78
5	P	2	FUC	C1-O5-C5	-5.03	101.38	112.78
4	M	1	NAG	C2-N2-C7	5.01	130.04	122.90
4	M	1	NAG	O3-C3-C2	-4.79	99.56	109.47
4	Q	1	NAG	C8-C7-N2	4.78	124.19	116.10
5	P	2	FUC	O5-C5-C6	4.61	117.26	107.33
4	O	1	NAG	O7-C7-C8	-4.59	113.53	122.06
4	Q	1	NAG	O5-C5-C6	-4.57	100.04	107.20
5	N	1	NAG	C1-O5-C5	-4.57	106.00	112.19
4	Q	2	NAG	C2-N2-C7	-4.44	116.58	122.90
5	R	2	FUC	C6-C5-C4	-4.35	105.04	113.07
4	M	1	NAG	O7-C7-C8	-4.30	114.06	122.06
4	Q	1	NAG	O7-C7-C8	-4.27	114.12	122.06
5	N	2	FUC	C6-C5-C4	-4.25	105.22	113.07
4	Q	1	NAG	O4-C4-C3	4.09	119.81	110.35
4	O	1	NAG	O5-C5-C6	-4.08	100.81	107.20
4	O	1	NAG	O3-C3-C2	-4.04	101.10	109.47
4	Q	1	NAG	O3-C3-C2	-3.96	101.27	109.47
4	O	2	NAG	C2-N2-C7	-3.94	117.29	122.90
4	Q	1	NAG	O3-C3-C4	3.77	119.06	110.35
4	O	1	NAG	C1-C2-N2	3.66	116.74	110.49
5	N	1	NAG	C4-C3-C2	3.59	116.29	111.02
4	M	1	NAG	C4-C3-C2	3.59	116.28	111.02
5	R	1	NAG	C1-O5-C5	-3.59	107.33	112.19
4	M	1	NAG	O4-C4-C3	3.59	118.64	110.35
5	S	1	NAG	C1-O5-C5	-3.47	107.49	112.19
4	O	1	NAG	O4-C4-C3	3.38	118.17	110.35
5	P	1	NAG	C1-O5-C5	-3.36	107.64	112.19
5	P	1	NAG	C4-C3-C2	3.33	115.90	111.02
5	P	2	FUC	C6-C5-C4	-3.29	107.00	113.07
4	O	1	NAG	C1-O5-C5	-3.19	107.87	112.19
4	O	1	NAG	C4-C3-C2	3.11	115.58	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	1	NAG	C8-C7-N2	3.04	121.25	116.10
5	R	1	NAG	C4-C3-C2	3.03	115.47	111.02
5	R	2	FUC	O2-C2-C1	2.88	115.05	109.15
4	Q	2	NAG	C1-O5-C5	-2.79	108.41	112.19
4	O	1	NAG	C8-C7-N2	2.78	120.80	116.10
5	N	1	NAG	O3-C3-C2	-2.75	103.78	109.47
5	P	1	NAG	C8-C7-N2	2.74	120.73	116.10
4	M	1	NAG	C1-O5-C5	-2.56	108.72	112.19
4	O	1	NAG	O3-C3-C4	2.49	116.10	110.35
4	M	1	NAG	O3-C3-C4	2.48	116.07	110.35
4	M	1	NAG	C1-C2-N2	2.47	114.71	110.49
4	O	2	NAG	C4-C3-C2	2.46	114.63	111.02
5	R	1	NAG	O4-C4-C5	2.40	115.25	109.30
5	S	1	NAG	C8-C7-N2	2.34	120.06	116.10
4	Q	1	NAG	C1-O5-C5	-2.32	109.05	112.19
4	O	2	NAG	O7-C7-N2	-2.28	117.77	121.95
4	Q	1	NAG	C4-C3-C2	2.27	114.34	111.02
5	S	2	FUC	C1-O5-C5	-2.26	107.66	112.78
5	P	1	NAG	O5-C1-C2	2.25	114.84	111.29
5	R	1	NAG	O5-C5-C4	2.19	116.16	110.83
5	R	2	FUC	O5-C1-C2	2.19	114.14	110.77
5	N	1	NAG	O4-C4-C5	2.17	114.68	109.30
4	O	1	NAG	C6-C5-C4	2.14	118.02	113.00
4	M	2	NAG	C1-O5-C5	-2.09	109.36	112.19
4	M	2	NAG	O7-C7-N2	-2.07	118.15	121.95
5	N	2	FUC	O2-C2-C1	2.06	113.37	109.15
5	P	2	FUC	O2-C2-C1	2.06	113.36	109.15
5	N	1	NAG	O5-C5-C4	2.05	115.81	110.83
5	P	1	NAG	O6-C6-C5	2.03	118.24	111.29
4	O	1	NAG	O7-C7-N2	2.02	125.67	121.95

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1	NAG	C3-C2-N2-C7
4	O	1	NAG	C3-C2-N2-C7
4	Q	1	NAG	C3-C2-N2-C7
4	O	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	Q	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6

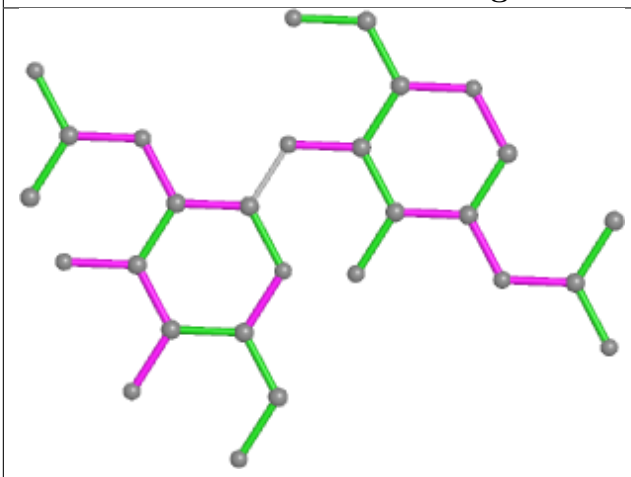
There are no ring outliers.

9 monomers are involved in 10 short contacts:

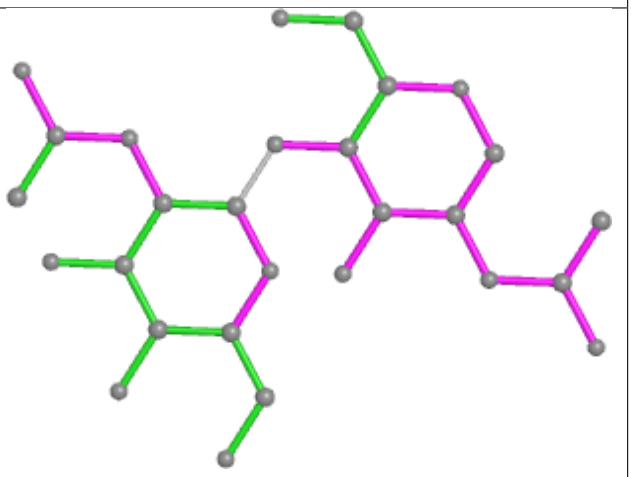
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1	NAG	1	0
4	O	1	NAG	1	0
4	Q	1	NAG	1	0
4	M	2	NAG	1	0
4	O	2	NAG	1	0
5	S	2	FUC	4	0
5	S	1	NAG	1	0
5	P	2	FUC	2	0
4	Q	2	NAG	1	0

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

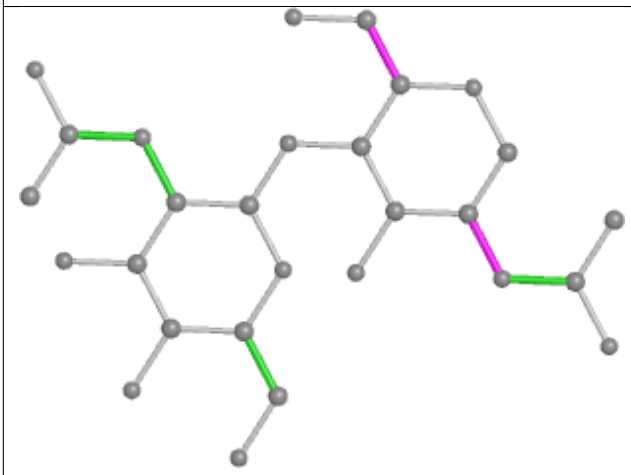
Oligosaccharide Chain M



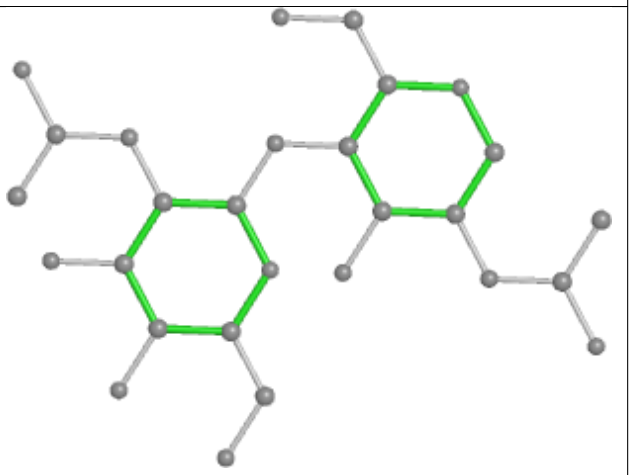
Bond lengths



Bond angles

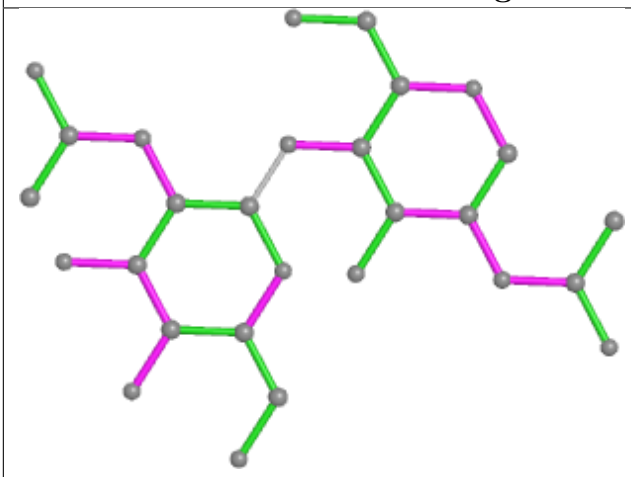


Torsions

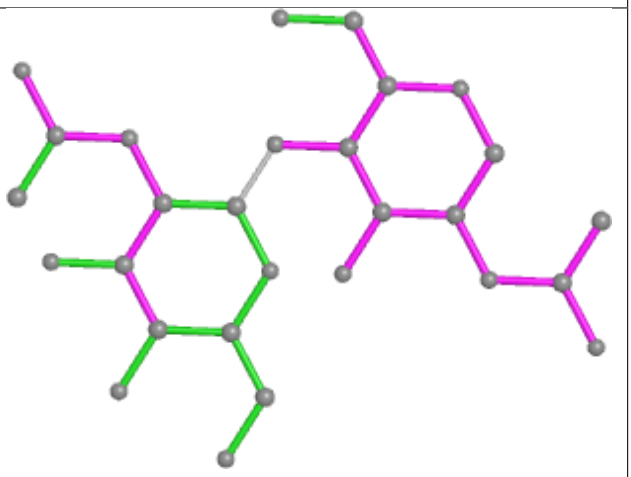


Rings

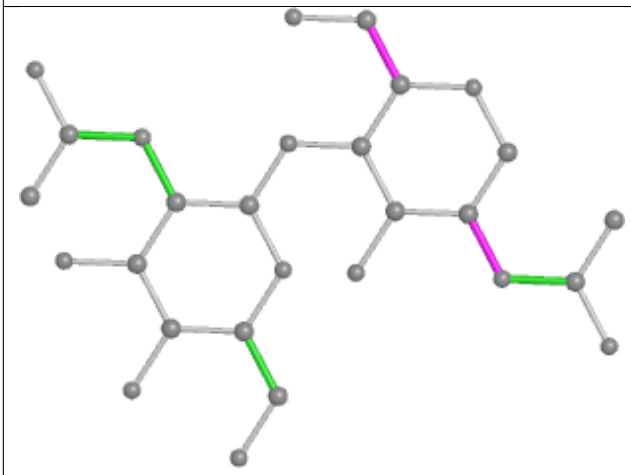
Oligosaccharide Chain O



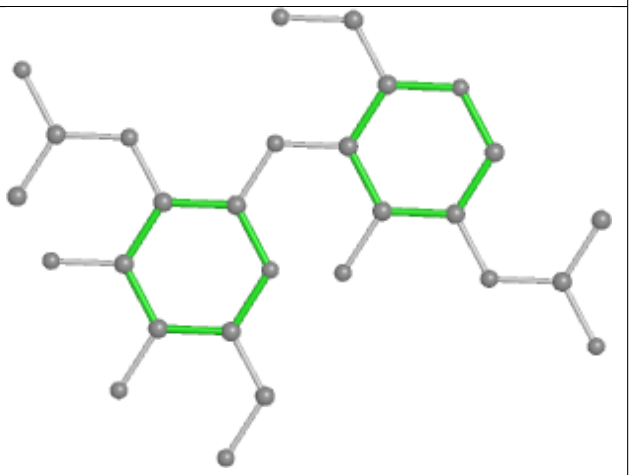
Bond lengths



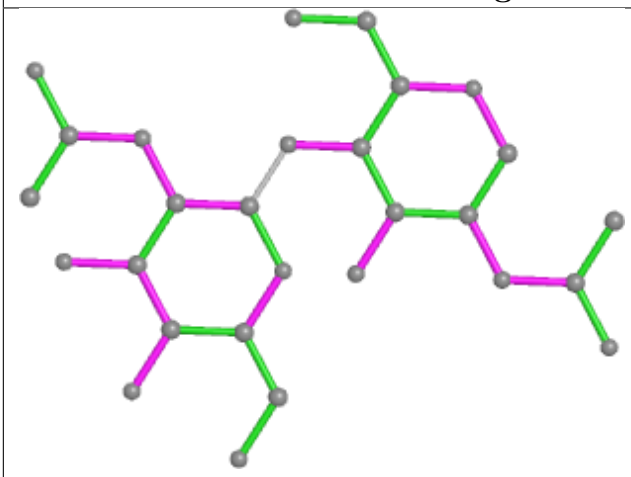
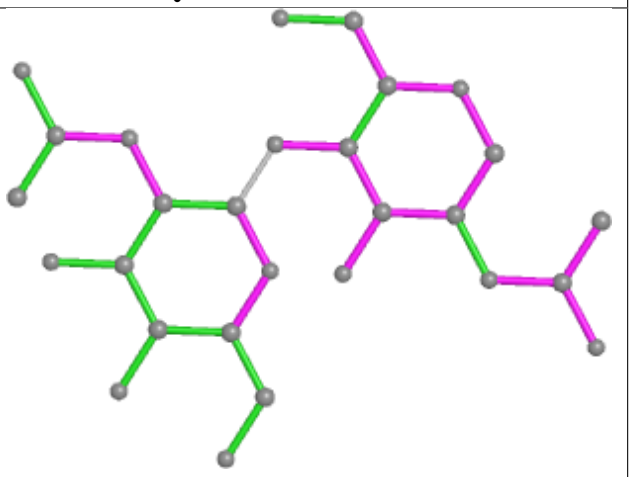
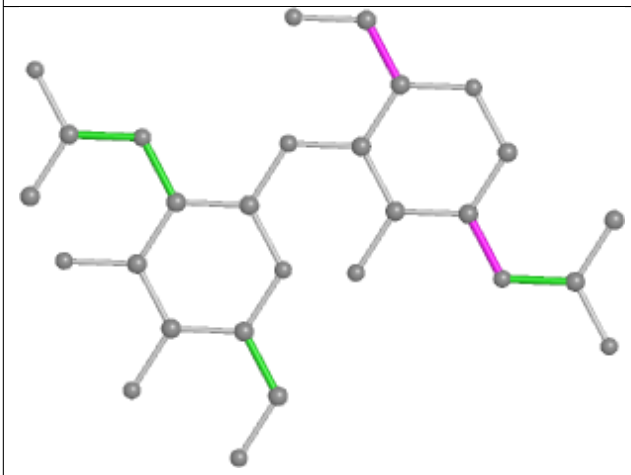
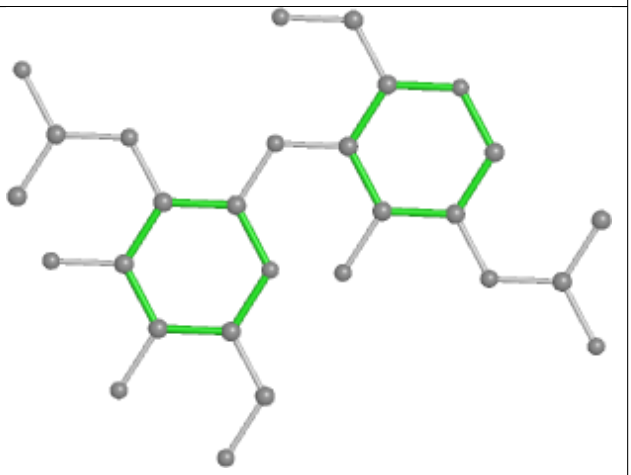
Bond angles

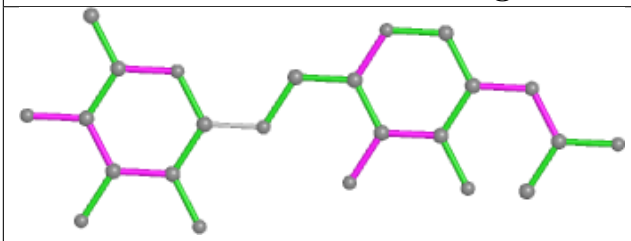
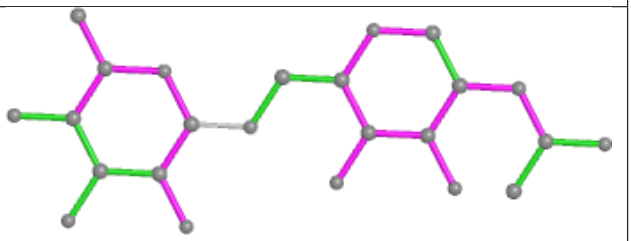
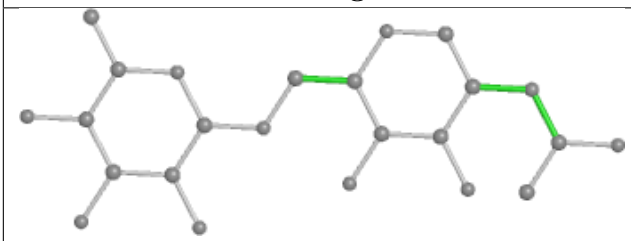
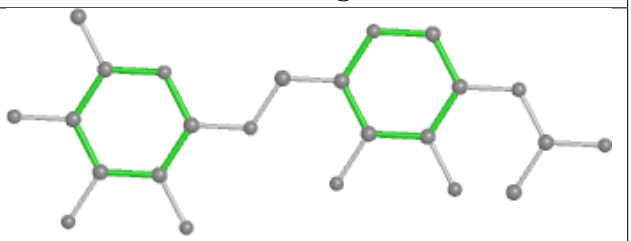


Torsions

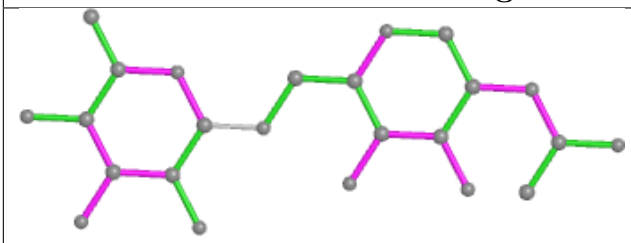


Rings

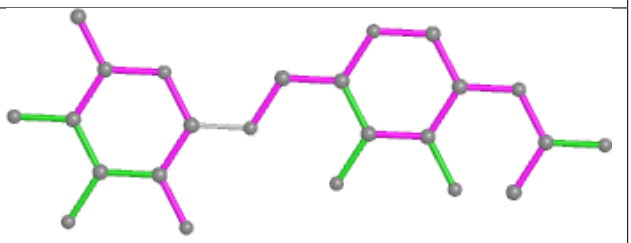
Oligosaccharide Chain Q	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

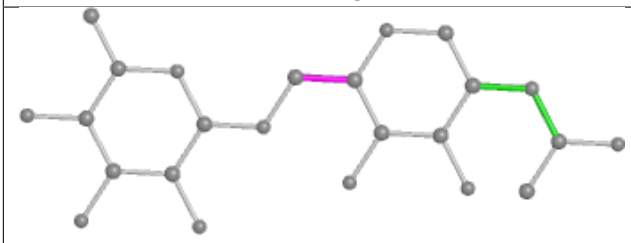
Oligosaccharide Chain P



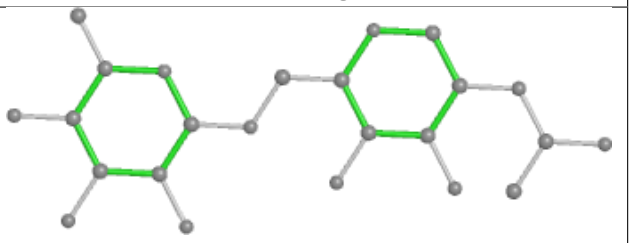
Bond lengths



Bond angles

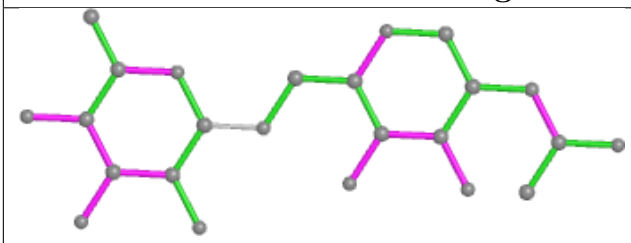


Torsions

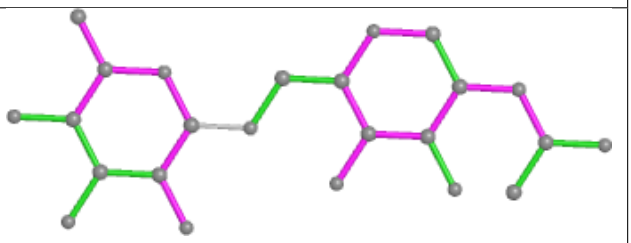


Rings

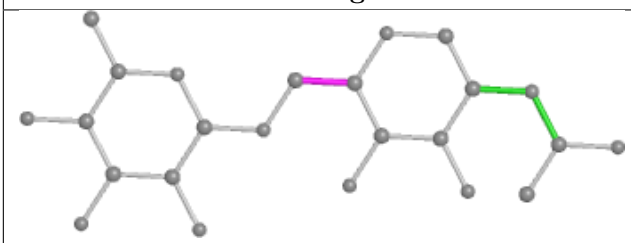
Oligosaccharide Chain R



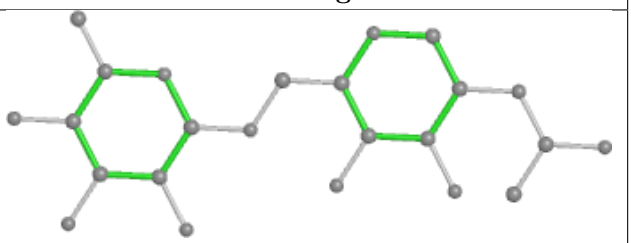
Bond lengths



Bond angles

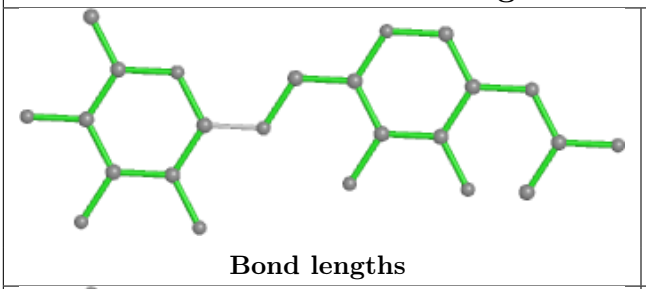


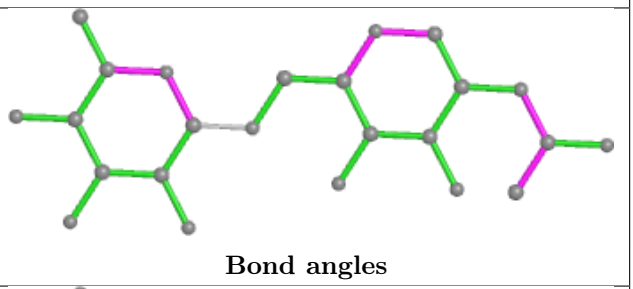
Torsions

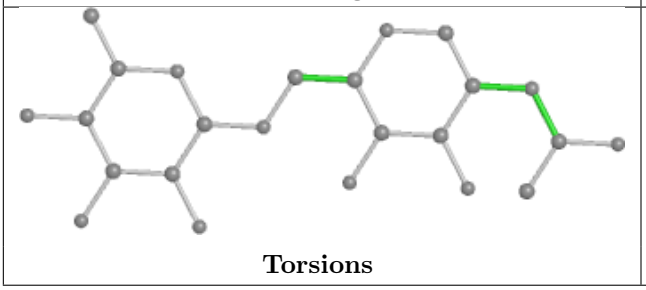


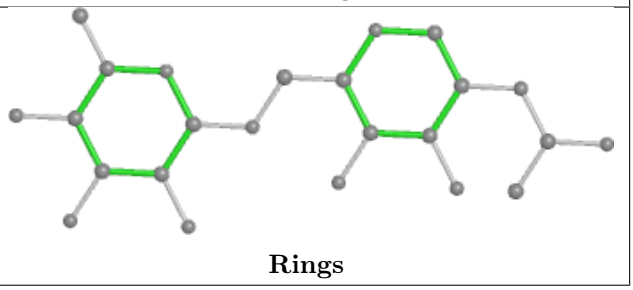
Rings

Oligosaccharide Chain S


Bond lengths


Bond angles


Torsions


Rings

5.6 Ligand geometry (i)

24 ligands 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	$\#\|Z\| > 2$
8	NAG	L	1002	3	14,14,15	0.42	0	17,19,21	1.38	2 (11%)
8	NAG	C	1003	3	14,14,15	2.19	5 (35%)	17,19,21	2.13	7 (41%)
7	OXY	J	202	6	1,1,1	0.15	0	-		
7	OXY	G	202	6	1,1,1	0.17	0	-		
6	HEM	D	201	7,1	41,50,50	1.86	8 (19%)	45,82,82	1.68	9 (20%)
6	HEM	G	201	7,1	41,50,50	1.84	9 (21%)	45,82,82	1.77	7 (15%)
7	OXY	E	202	6	1,1,1	0.15	0	-		
8	NAG	F	1004	3	14,14,15	1.80	5 (35%)	17,19,21	1.62	2 (11%)
7	OXY	H	202	6	1,1,1	0.12	0	-		
7	OXY	D	202	6	1,1,1	0.19	0	-		
8	NAG	L	1001	3	14,14,15	2.47	7 (50%)	17,19,21	2.12	3 (17%)
7	OXY	K	202	6	1,1,1	0.11	0	-		
6	HEM	A	201	7,1	41,50,50	1.92	8 (19%)	45,82,82	1.79	9 (20%)
8	NAG	I	1003	3	14,14,15	2.09	5 (35%)	17,19,21	1.58	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	OXY	B	202	6	1,1,1	0.15	0	-		
6	HEM	H	201	2,7	41,50,50	1.95	6 (14%)	45,82,82	1.96	8 (17%)
6	HEM	K	201	2,7	41,50,50	2.01	7 (17%)	45,82,82	1.94	10 (22%)
8	NAG	C	1004	3	14,14,15	2.48	6 (42%)	17,19,21	2.64	9 (52%)
6	HEM	J	201	7,1	41,50,50	1.89	7 (17%)	45,82,82	1.74	6 (13%)
7	OXY	A	202	6	1,1,1	0.16	0	-		
6	HEM	E	201	2,7	41,50,50	1.92	7 (17%)	45,82,82	1.88	10 (22%)
6	HEM	B	201	2,7	41,50,50	2.01	8 (19%)	45,82,82	1.91	10 (22%)
8	NAG	F	1003	3	14,14,15	2.28	6 (42%)	17,19,21	2.23	4 (23%)
8	NAG	I	1004	3	14,14,15	1.87	5 (35%)	17,19,21	1.94	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	L	1002	3	-	0/6/23/26	0/1/1/1
8	NAG	C	1003	3	-	0/6/23/26	0/1/1/1
6	HEM	A	201	7,1	-	2/12/54/54	-
6	HEM	E	201	2,7	-	6/12/54/54	-
8	NAG	I	1003	3	-	0/6/23/26	0/1/1/1
6	HEM	D	201	7,1	-	2/12/54/54	-
6	HEM	B	201	2,7	-	6/12/54/54	-
8	NAG	L	1001	3	-	3/6/23/26	0/1/1/1
6	HEM	H	201	2,7	-	6/12/54/54	-
6	HEM	K	201	2,7	-	5/12/54/54	-
8	NAG	C	1004	3	-	3/6/23/26	0/1/1/1
8	NAG	F	1003	3	-	0/6/23/26	0/1/1/1
6	HEM	G	201	7,1	-	2/12/54/54	-
8	NAG	F	1004	3	-	0/6/23/26	0/1/1/1
6	HEM	J	201	7,1	-	2/12/54/54	-
8	NAG	I	1004	3	-	0/6/23/26	0/1/1/1

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	201	HEM	C3D-C2D	8.42	1.54	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	201	HEM	C3D-C2D	8.00	1.53	1.36
6	A	201	HEM	C3D-C2D	7.93	1.53	1.36
6	H	201	HEM	C3D-C2D	7.79	1.53	1.36
6	J	201	HEM	C3D-C2D	7.75	1.53	1.36
6	E	201	HEM	C3D-C2D	7.63	1.53	1.36
6	D	201	HEM	C3D-C2D	7.50	1.52	1.36
6	G	201	HEM	C3D-C2D	7.43	1.52	1.36
8	C	1004	NAG	O5-C5	4.81	1.53	1.43
8	C	1003	NAG	O5-C5	4.45	1.52	1.43
8	I	1003	NAG	O5-C5	4.44	1.52	1.43
8	L	1001	NAG	C7-N2	4.41	1.49	1.34
6	B	201	HEM	C3C-CAC	4.40	1.56	1.47
8	F	1003	NAG	O5-C5	4.39	1.52	1.43
6	H	201	HEM	C3C-CAC	4.18	1.56	1.47
8	C	1004	NAG	C7-N2	4.11	1.48	1.34
6	E	201	HEM	C3C-CAC	4.04	1.56	1.47
8	C	1003	NAG	C7-N2	3.94	1.47	1.34
6	K	201	HEM	C3C-CAC	3.90	1.55	1.47
8	L	1001	NAG	O5-C5	3.81	1.51	1.43
8	L	1001	NAG	C2-N2	3.74	1.52	1.46
6	J	201	HEM	C3C-C2C	-3.71	1.35	1.40
8	F	1003	NAG	C7-N2	3.70	1.47	1.34
6	H	201	HEM	C3C-C2C	-3.70	1.35	1.40
6	B	201	HEM	C3C-C2C	-3.69	1.35	1.40
6	J	201	HEM	C3C-CAC	3.69	1.55	1.47
6	A	201	HEM	C3C-CAC	3.69	1.55	1.47
6	E	201	HEM	C3C-C2C	-3.67	1.35	1.40
8	I	1003	NAG	C7-N2	3.63	1.46	1.34
6	D	201	HEM	C3C-CAC	3.57	1.55	1.47
6	G	201	HEM	C3C-CAC	3.56	1.55	1.47
8	C	1004	NAG	O4-C4	3.51	1.51	1.43
6	D	201	HEM	C3C-C2C	-3.48	1.35	1.40
6	K	201	HEM	C3C-C2C	-3.48	1.35	1.40
6	A	201	HEM	C3C-C2C	-3.34	1.35	1.40
6	H	201	HEM	FE-ND	3.33	2.13	1.96
6	E	201	HEM	FE-ND	3.32	2.13	1.96
8	I	1004	NAG	C4-C3	-3.30	1.43	1.52
8	F	1003	NAG	C1-C2	3.25	1.57	1.52
8	I	1004	NAG	O5-C1	-3.25	1.38	1.43
6	K	201	HEM	CAB-C3B	3.23	1.56	1.47
8	I	1004	NAG	C7-N2	3.18	1.45	1.34
6	K	201	HEM	FE-NB	3.13	2.12	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	201	HEM	C3C-C2C	-3.11	1.36	1.40
6	A	201	HEM	FE-ND	3.09	2.12	1.96
6	B	201	HEM	CAB-C3B	3.05	1.55	1.47
6	D	201	HEM	FE-ND	3.04	2.11	1.96
8	L	1001	NAG	C4-C3	-3.03	1.44	1.52
8	C	1003	NAG	C2-N2	3.03	1.51	1.46
8	F	1004	NAG	O5-C1	-2.99	1.38	1.43
8	I	1003	NAG	C2-N2	2.97	1.51	1.46
8	F	1004	NAG	O5-C5	2.96	1.49	1.43
6	H	201	HEM	CAB-C3B	2.95	1.55	1.47
6	E	201	HEM	CAB-C3B	2.92	1.55	1.47
8	C	1004	NAG	C4-C3	-2.86	1.45	1.52
8	C	1004	NAG	O3-C3	2.73	1.49	1.43
6	J	201	HEM	CAB-C3B	2.73	1.54	1.47
8	F	1003	NAG	C4-C3	-2.70	1.45	1.52
6	B	201	HEM	FE-NB	2.68	2.10	1.96
6	J	201	HEM	FE-NB	2.66	2.10	1.96
8	L	1001	NAG	O4-C4	2.62	1.49	1.43
8	I	1003	NAG	O3-C3	2.60	1.49	1.43
6	G	201	HEM	FE-ND	2.59	2.09	1.96
8	C	1003	NAG	C4-C3	-2.58	1.45	1.52
6	D	201	HEM	O1A-CGA	2.53	1.30	1.22
6	E	201	HEM	CAA-C2A	2.52	1.55	1.52
6	G	201	HEM	CAB-C3B	2.48	1.54	1.47
6	A	201	HEM	O1A-CGA	2.46	1.30	1.22
6	G	201	HEM	FE-NB	2.44	2.08	1.96
8	F	1003	NAG	C2-N2	2.44	1.50	1.46
8	F	1004	NAG	C7-N2	2.43	1.42	1.34
8	F	1003	NAG	O3-C3	2.42	1.48	1.43
6	B	201	HEM	CAA-C2A	2.39	1.55	1.52
6	D	201	HEM	CAB-C3B	2.38	1.53	1.47
8	I	1004	NAG	O5-C5	2.36	1.48	1.43
8	C	1004	NAG	C3-C2	-2.35	1.47	1.52
6	H	201	HEM	CAA-C2A	2.35	1.55	1.52
8	L	1001	NAG	C3-C2	-2.32	1.47	1.52
6	K	201	HEM	CMB-C2B	2.32	1.55	1.50
6	K	201	HEM	FE-ND	2.29	2.08	1.96
8	I	1003	NAG	C4-C3	-2.28	1.46	1.52
6	A	201	HEM	CAB-C3B	2.28	1.53	1.47
6	B	201	HEM	FE-ND	2.27	2.08	1.96
6	J	201	HEM	FE-ND	2.26	2.08	1.96
8	L	1001	NAG	O3-C3	2.26	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	201	HEM	CMC-C2C	2.24	1.56	1.51
8	F	1004	NAG	O4-C4	2.23	1.48	1.43
8	F	1004	NAG	C4-C3	-2.21	1.46	1.52
8	C	1003	NAG	O3-C3	2.19	1.48	1.43
6	E	201	HEM	CMB-C2B	2.19	1.55	1.50
8	I	1004	NAG	O4-C4	2.19	1.48	1.43
6	G	201	HEM	CMB-C2B	2.14	1.55	1.50
6	D	201	HEM	O1D-CGD	2.12	1.29	1.22
6	G	201	HEM	O1A-CGA	2.10	1.29	1.22
6	D	201	HEM	CMB-C2B	2.09	1.55	1.50
6	A	201	HEM	CMC-C2C	2.08	1.56	1.51
6	B	201	HEM	C1A-NA	2.06	1.40	1.36
6	J	201	HEM	CMB-C2B	2.04	1.55	1.50
6	A	201	HEM	CMB-C2B	2.03	1.55	1.50

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	201	HEM	C4D-ND-C1D	7.50	112.82	105.07
8	F	1003	NAG	O5-C1-C2	-7.04	100.17	111.29
6	H	201	HEM	C4D-ND-C1D	6.69	111.99	105.07
6	B	201	HEM	C4D-ND-C1D	6.44	111.73	105.07
6	E	201	HEM	C4D-ND-C1D	6.37	111.66	105.07
6	A	201	HEM	C4D-ND-C1D	6.31	111.59	105.07
6	J	201	HEM	C4D-ND-C1D	6.29	111.56	105.07
6	G	201	HEM	C4D-ND-C1D	6.08	111.35	105.07
6	D	201	HEM	C4D-ND-C1D	5.98	111.25	105.07
8	C	1004	NAG	O5-C5-C6	5.51	115.84	107.20
8	C	1003	NAG	C2-N2-C7	-5.40	115.21	122.90
8	L	1001	NAG	C1-O5-C5	-5.27	105.06	112.19
8	C	1004	NAG	C2-N2-C7	4.66	129.53	122.90
8	I	1004	NAG	C8-C7-N2	4.64	123.95	116.10
6	H	201	HEM	C4C-CHD-C1D	4.34	128.29	122.56
8	L	1001	NAG	C2-N2-C7	4.08	128.71	122.90
6	K	201	HEM	C4B-CHC-C1C	4.07	127.94	122.56
8	C	1004	NAG	C4-C3-C2	4.07	116.98	111.02
6	B	201	HEM	C4C-CHD-C1D	4.06	127.91	122.56
8	I	1003	NAG	C2-N2-C7	-4.03	117.16	122.90
6	B	201	HEM	C4B-CHC-C1C	3.84	127.62	122.56
6	B	201	HEM	C4A-C3A-C2A	3.80	109.64	107.00
8	F	1004	NAG	C1-C2-N2	-3.78	104.03	110.49
6	E	201	HEM	C4C-CHD-C1D	3.76	127.52	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	1001	NAG	O7-C7-C8	-3.60	115.37	122.06
6	A	201	HEM	CBD-CAD-C3D	-3.57	102.71	112.63
6	H	201	HEM	C4B-CHC-C1C	3.53	127.22	122.56
6	H	201	HEM	C1B-NB-C4B	3.48	108.67	105.07
6	E	201	HEM	C4B-CHC-C1C	3.42	127.07	122.56
6	A	201	HEM	C4C-CHD-C1D	3.42	127.07	122.56
8	L	1002	NAG	C1-O5-C5	-3.36	107.64	112.19
8	F	1003	NAG	C2-N2-C7	-3.30	118.20	122.90
8	I	1004	NAG	O6-C6-C5	3.28	122.53	111.29
6	G	201	HEM	CBD-CAD-C3D	-3.27	103.53	112.63
6	D	201	HEM	C4C-CHD-C1D	3.23	126.82	122.56
8	I	1004	NAG	O7-C7-C8	-3.23	116.06	122.06
6	G	201	HEM	C1B-NB-C4B	3.22	108.40	105.07
6	A	201	HEM	C4B-CHC-C1C	3.19	126.76	122.56
8	F	1003	NAG	O5-C5-C6	3.17	112.17	107.20
6	J	201	HEM	C4C-CHD-C1D	3.16	126.72	122.56
6	J	201	HEM	CBD-CAD-C3D	-3.14	103.91	112.63
8	C	1003	NAG	O5-C1-C2	3.10	116.19	111.29
8	F	1004	NAG	C8-C7-N2	3.10	121.35	116.10
6	E	201	HEM	C1B-NB-C4B	3.10	108.27	105.07
8	C	1004	NAG	O7-C7-C8	-3.08	116.34	122.06
6	A	201	HEM	CAA-CBA-CGA	-3.08	105.14	113.76
6	K	201	HEM	C1B-NB-C4B	3.06	108.23	105.07
6	H	201	HEM	C4A-C3A-C2A	3.05	109.11	107.00
6	D	201	HEM	C4B-CHC-C1C	3.03	126.56	122.56
6	D	201	HEM	CBD-CAD-C3D	-3.02	104.23	112.63
8	I	1004	NAG	C1-C2-N2	-3.00	105.36	110.49
6	B	201	HEM	C1B-NB-C4B	3.00	108.17	105.07
6	J	201	HEM	C4B-CHC-C1C	2.99	126.50	122.56
6	E	201	HEM	CHC-C4B-NB	2.98	127.67	124.43
6	H	201	HEM	CHC-C4B-NB	2.98	127.67	124.43
6	H	201	HEM	CMA-C3A-C4A	-2.96	123.91	128.46
6	G	201	HEM	C4B-CHC-C1C	2.93	126.43	122.56
6	G	201	HEM	C4C-CHD-C1D	2.89	126.37	122.56
8	C	1004	NAG	C6-C5-C4	-2.83	106.37	113.00
6	J	201	HEM	C1B-NB-C4B	2.83	108.00	105.07
6	K	201	HEM	C4C-CHD-C1D	2.82	126.29	122.56
6	K	201	HEM	CAD-CBD-CGD	-2.72	107.75	113.60
8	C	1004	NAG	O7-C7-N2	2.71	126.94	121.95
6	B	201	HEM	CHC-C4B-NB	2.68	127.34	124.43
6	G	201	HEM	CAA-CBA-CGA	-2.67	106.26	113.76
6	E	201	HEM	CMA-C3A-C4A	-2.67	124.36	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1004	NAG	O6-C6-C5	2.67	120.45	111.29
8	C	1004	NAG	O4-C4-C5	2.66	115.91	109.30
6	E	201	HEM	C4A-C3A-C2A	2.62	108.82	107.00
6	K	201	HEM	CMC-C2C-C3C	2.61	129.56	124.68
6	B	201	HEM	CMA-C3A-C4A	-2.60	124.46	128.46
6	J	201	HEM	CAA-CBA-CGA	-2.58	106.52	113.76
8	I	1003	NAG	O3-C3-C4	2.56	116.27	110.35
6	K	201	HEM	CBA-CAA-C2A	-2.55	108.26	112.62
8	I	1003	NAG	C1-O5-C5	-2.52	108.78	112.19
6	D	201	HEM	CAA-CBA-CGA	-2.52	106.70	113.76
8	C	1003	NAG	C8-C7-N2	2.51	120.35	116.10
6	E	201	HEM	CAD-C3D-C4D	2.49	129.01	124.66
8	C	1003	NAG	O3-C3-C2	-2.48	104.33	109.47
8	C	1003	NAG	C4-C3-C2	2.42	114.56	111.02
6	A	201	HEM	C4B-C3B-C2B	2.40	109.02	107.11
6	A	201	HEM	C1B-NB-C4B	2.37	107.52	105.07
6	G	201	HEM	C4B-C3B-C2B	2.35	108.98	107.11
8	L	1002	NAG	C8-C7-N2	2.34	120.07	116.10
6	K	201	HEM	CHA-C4D-ND	2.23	127.14	124.38
6	B	201	HEM	CAD-C3D-C4D	2.22	128.54	124.66
6	D	201	HEM	C1B-NB-C4B	2.20	107.35	105.07
8	C	1004	NAG	C1-C2-N2	-2.19	106.75	110.49
6	H	201	HEM	CAD-C3D-C4D	2.18	128.47	124.66
6	K	201	HEM	CHD-C1D-ND	2.16	126.78	124.43
6	E	201	HEM	CAD-CBD-CGD	-2.15	108.97	113.60
6	D	201	HEM	C1D-C2D-C3D	-2.13	104.72	106.96
6	A	201	HEM	CHC-C4B-NB	2.13	126.74	124.43
8	C	1003	NAG	C1-O5-C5	-2.11	109.34	112.19
8	C	1003	NAG	O3-C3-C4	2.08	115.17	110.35
6	D	201	HEM	O1A-CGA-CBA	-2.07	116.42	123.08
6	D	201	HEM	CMD-C2D-C1D	2.07	128.19	125.04
6	K	201	HEM	C3D-C4D-ND	-2.05	107.88	110.17
6	B	201	HEM	O2A-CGA-CBA	2.05	120.61	114.03
8	F	1003	NAG	O3-C3-C4	2.04	115.07	110.35
6	A	201	HEM	CAD-C3D-C4D	2.04	128.22	124.66
6	E	201	HEM	CMC-C2C-C3C	2.03	128.48	124.68
6	B	201	HEM	O2D-CGD-CBD	2.00	120.47	114.03

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	201	HEM	C1A-C2A-CAA-CBA
6	B	201	HEM	C3A-C2A-CAA-CBA
6	E	201	HEM	C1A-C2A-CAA-CBA
6	E	201	HEM	C3A-C2A-CAA-CBA
6	H	201	HEM	C1A-C2A-CAA-CBA
6	H	201	HEM	C3A-C2A-CAA-CBA
8	C	1004	NAG	C3-C2-N2-C7
8	L	1001	NAG	C3-C2-N2-C7
8	L	1001	NAG	O5-C5-C6-O6
6	K	201	HEM	C3D-CAD-CBD-CGD
8	C	1004	NAG	O5-C5-C6-O6
8	L	1001	NAG	C4-C5-C6-O6
6	B	201	HEM	C3D-CAD-CBD-CGD
6	E	201	HEM	C3D-CAD-CBD-CGD
6	H	201	HEM	C3D-CAD-CBD-CGD
6	E	201	HEM	C2A-CAA-CBA-CGA
6	H	201	HEM	C2A-CAA-CBA-CGA
6	B	201	HEM	C2A-CAA-CBA-CGA
6	K	201	HEM	C1A-C2A-CAA-CBA
6	B	201	HEM	CAD-CBD-CGD-O2D
8	C	1004	NAG	C4-C5-C6-O6
6	B	201	HEM	CAD-CBD-CGD-O1D
6	H	201	HEM	CAD-CBD-CGD-O1D
6	E	201	HEM	CAD-CBD-CGD-O2D
6	H	201	HEM	CAD-CBD-CGD-O2D
6	E	201	HEM	CAD-CBD-CGD-O1D
6	G	201	HEM	CAD-CBD-CGD-O1D
6	D	201	HEM	CAD-CBD-CGD-O1D
6	D	201	HEM	CAD-CBD-CGD-O2D
6	G	201	HEM	CAD-CBD-CGD-O2D
6	J	201	HEM	CAD-CBD-CGD-O1D
6	A	201	HEM	CAD-CBD-CGD-O1D
6	K	201	HEM	CAD-CBD-CGD-O1D
6	K	201	HEM	C2A-CAA-CBA-CGA
6	J	201	HEM	CAD-CBD-CGD-O2D
6	A	201	HEM	CAD-CBD-CGD-O2D
6	K	201	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	1002	NAG	1	0

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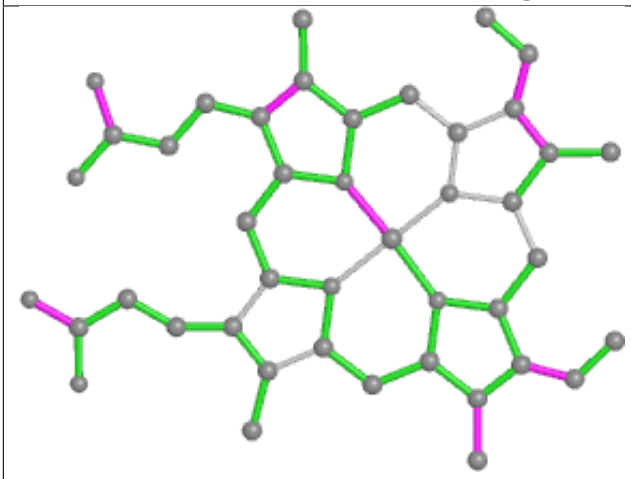
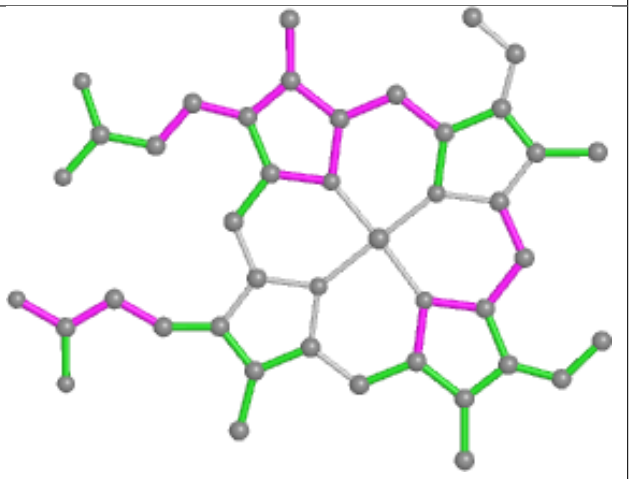
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1003	NAG	1	0
6	A	201	HEM	1	0
6	H	201	HEM	4	0
6	K	201	HEM	2	0
6	E	201	HEM	5	0
6	B	201	HEM	4	0

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.

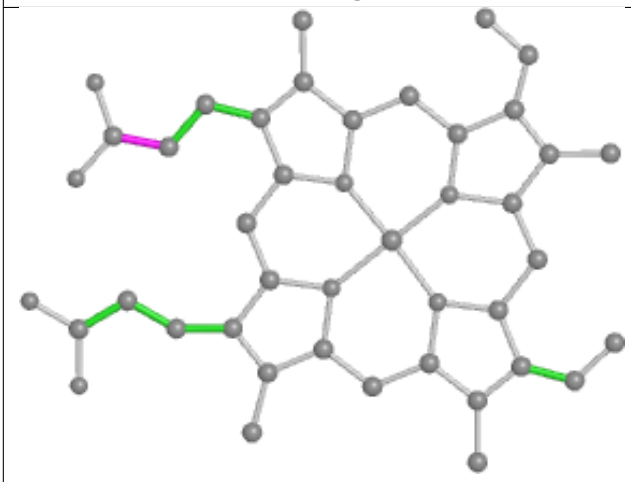
Ligand HEM D 201



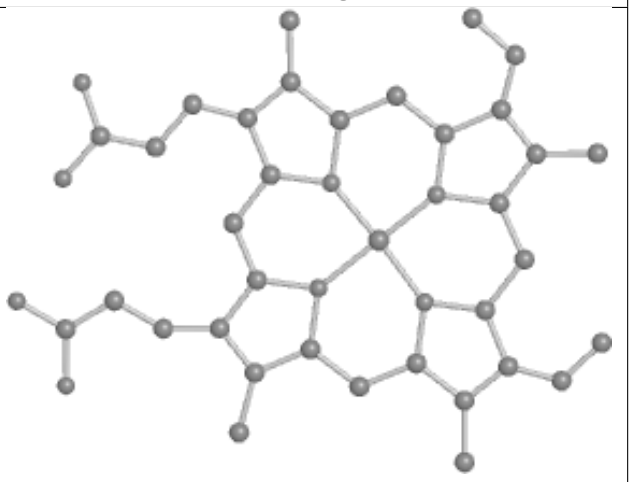
Bond lengths



Bond angles

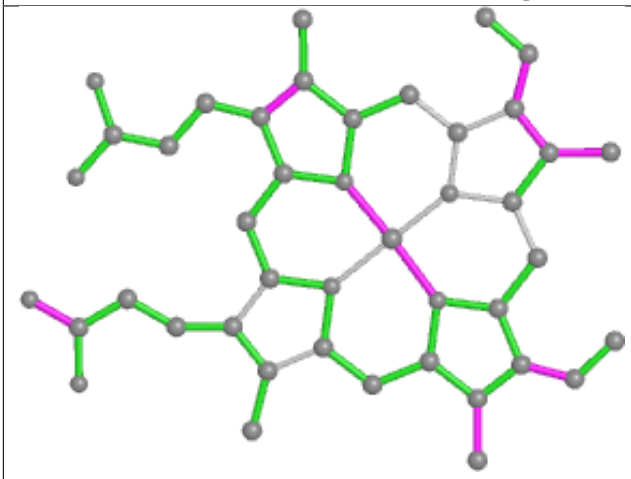


Torsions

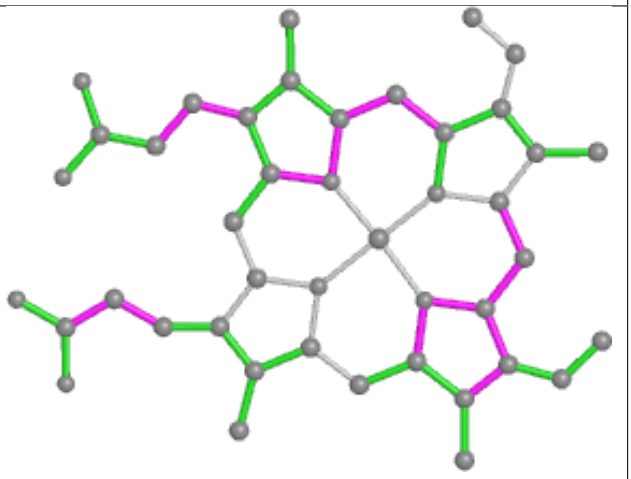


Rings

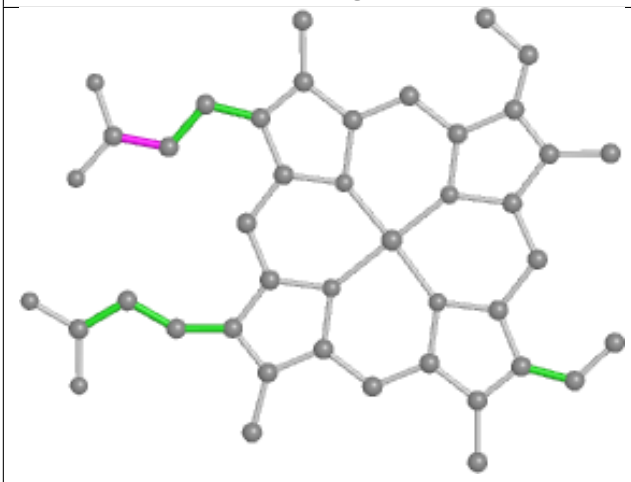
Ligand HEM G 201



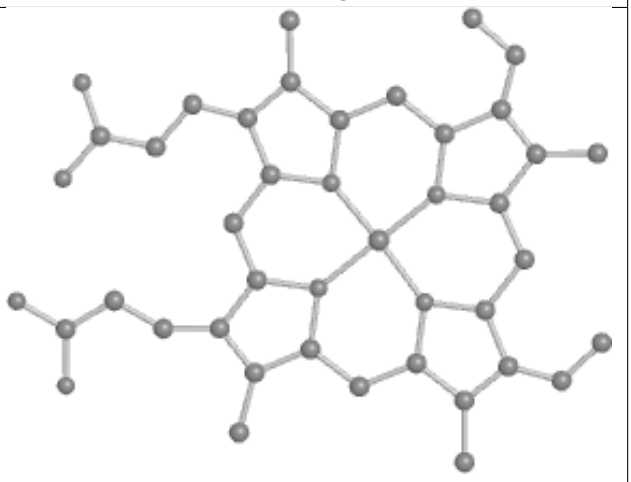
Bond lengths



Bond angles

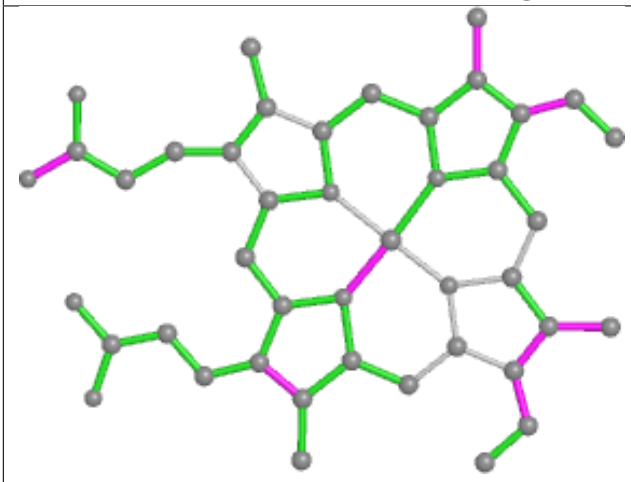


Torsions

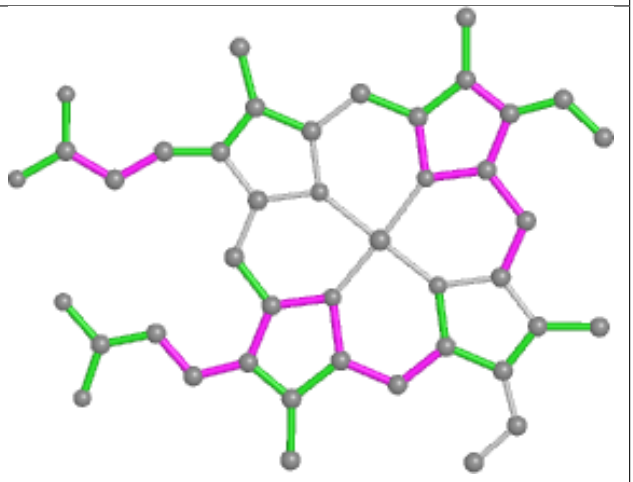


Rings

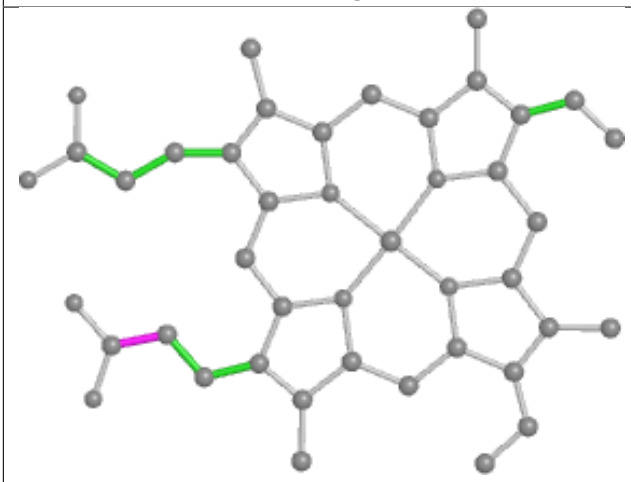
Ligand HEM A 201



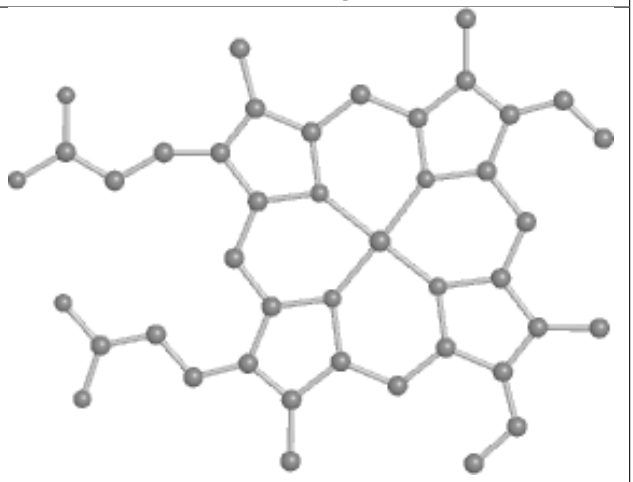
Bond lengths



Bond angles

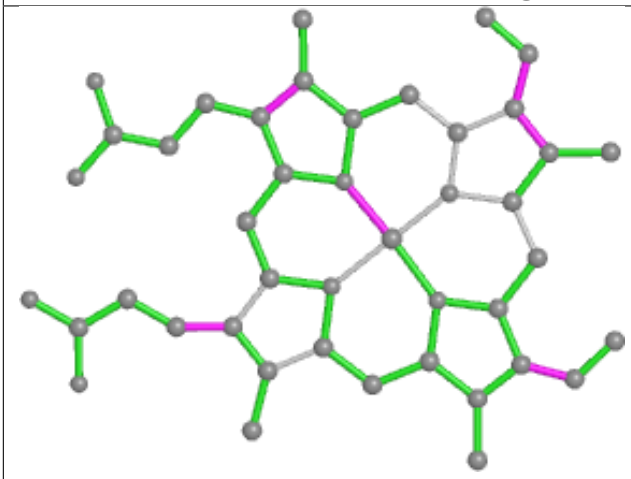


Torsions



Rings

Ligand HEM H 201



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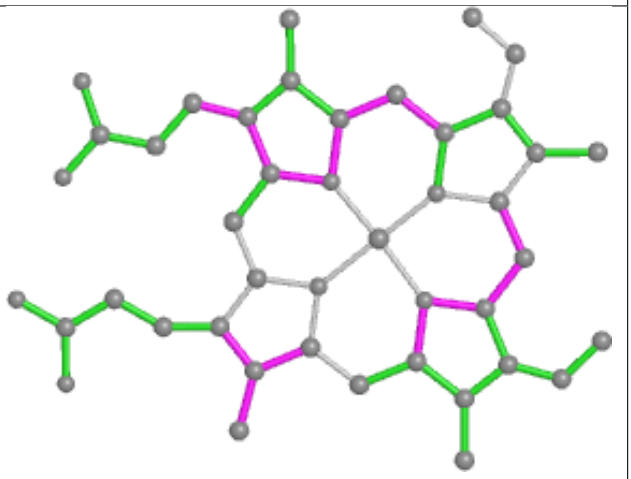
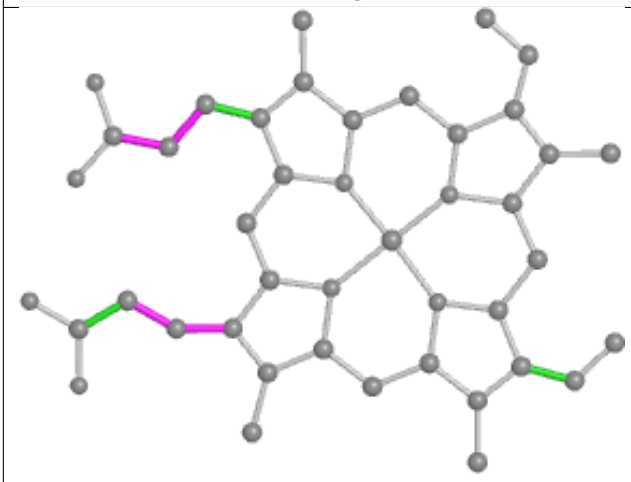


Bond angles



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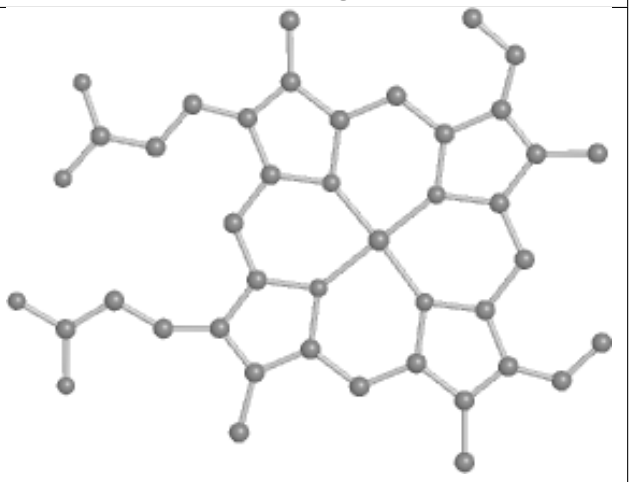
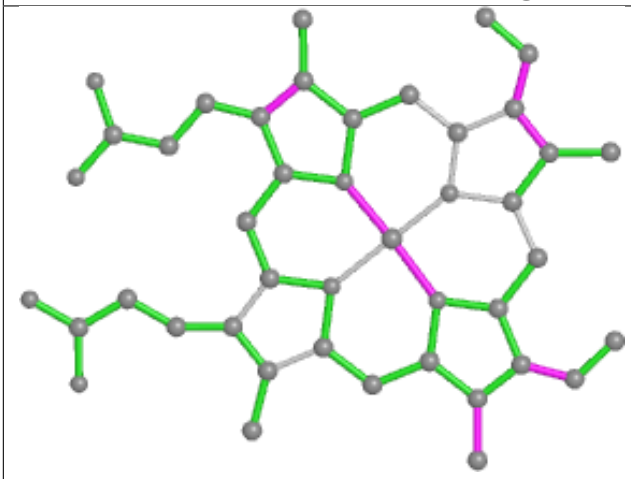
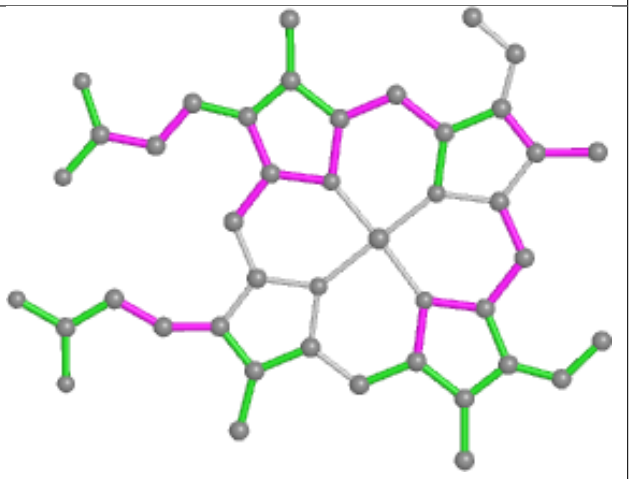


Rings

Ligand HEM K 201



Bond lengths



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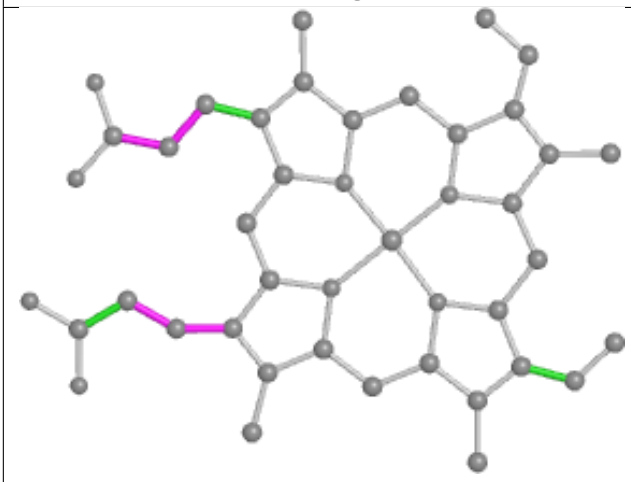

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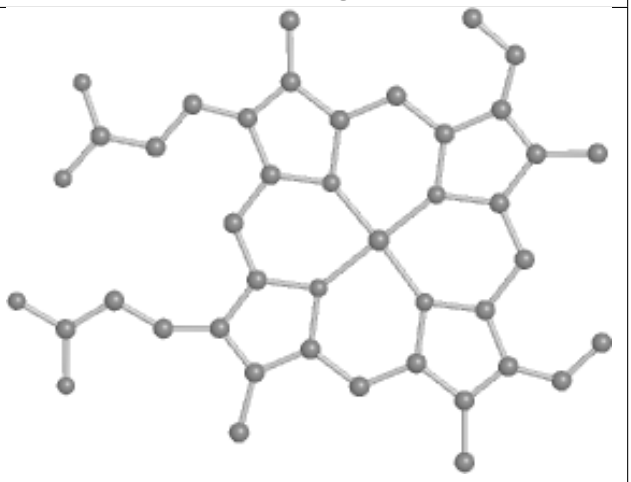
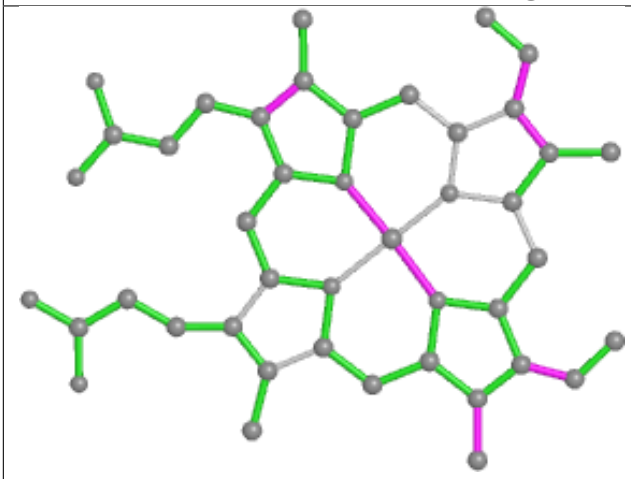


Rings

Ligand HEM J 201



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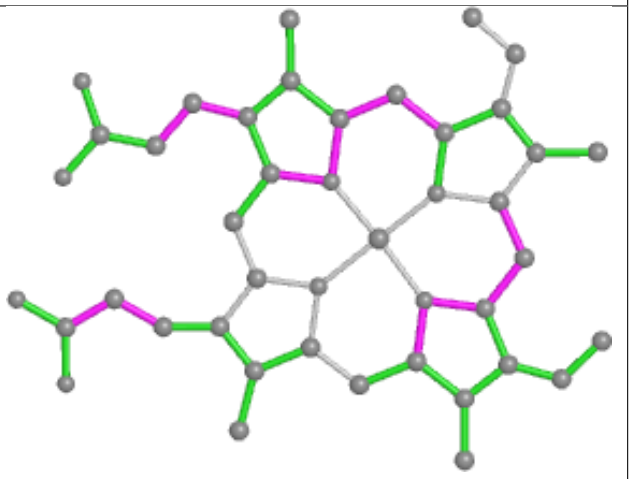
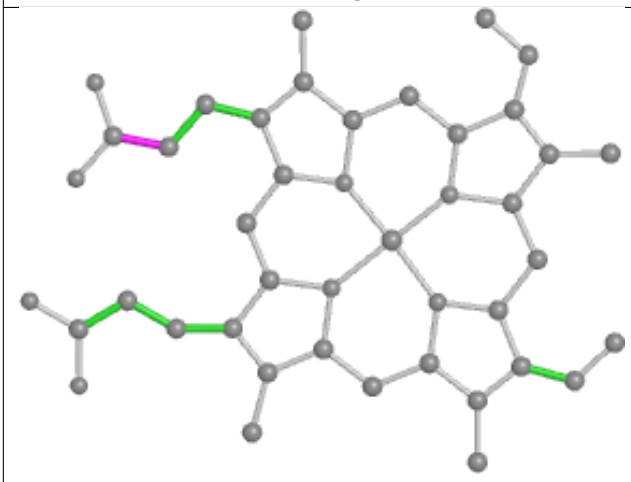


Bond angles



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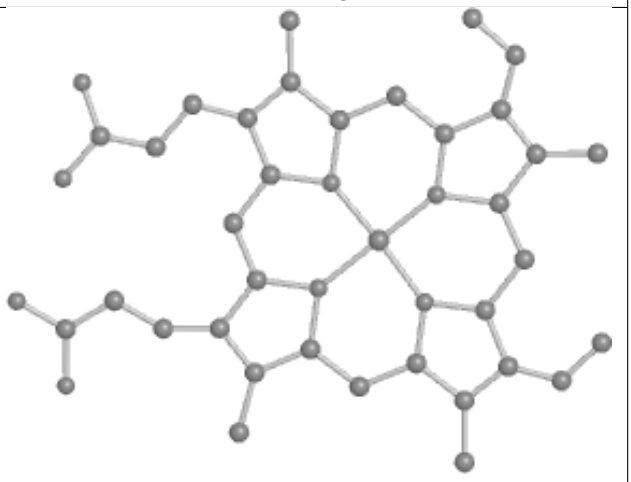

Rings

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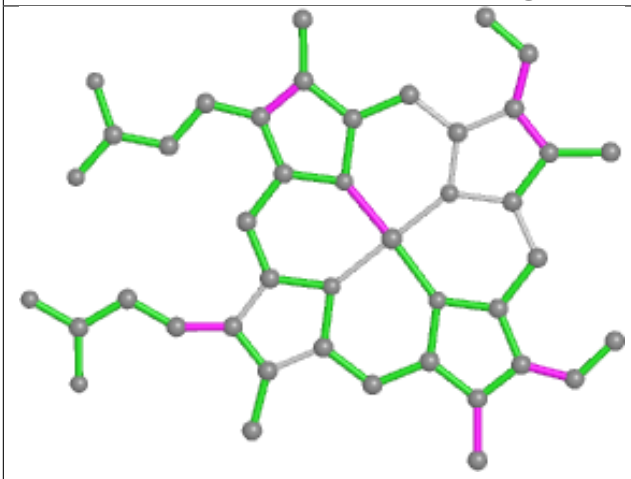
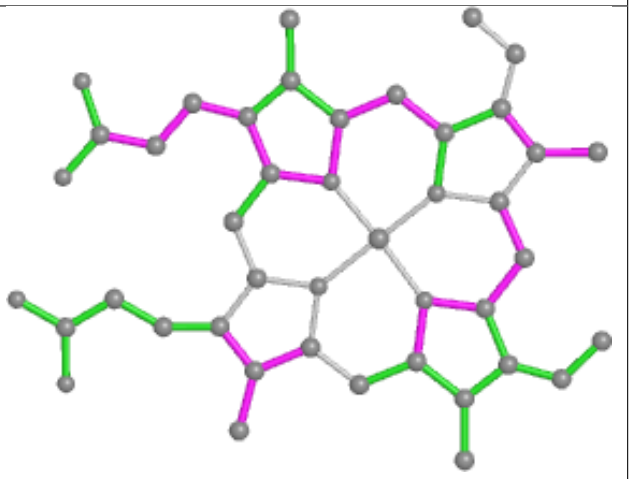
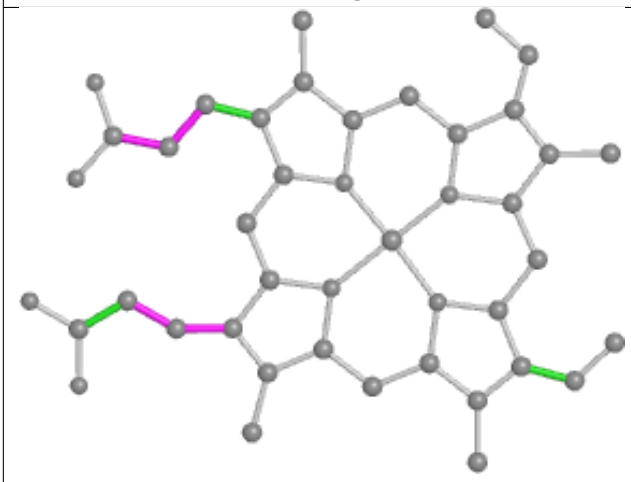


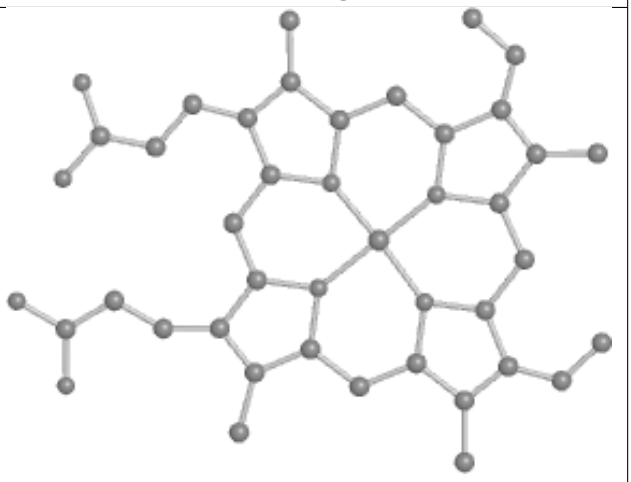
Bond lengths



Bond angles

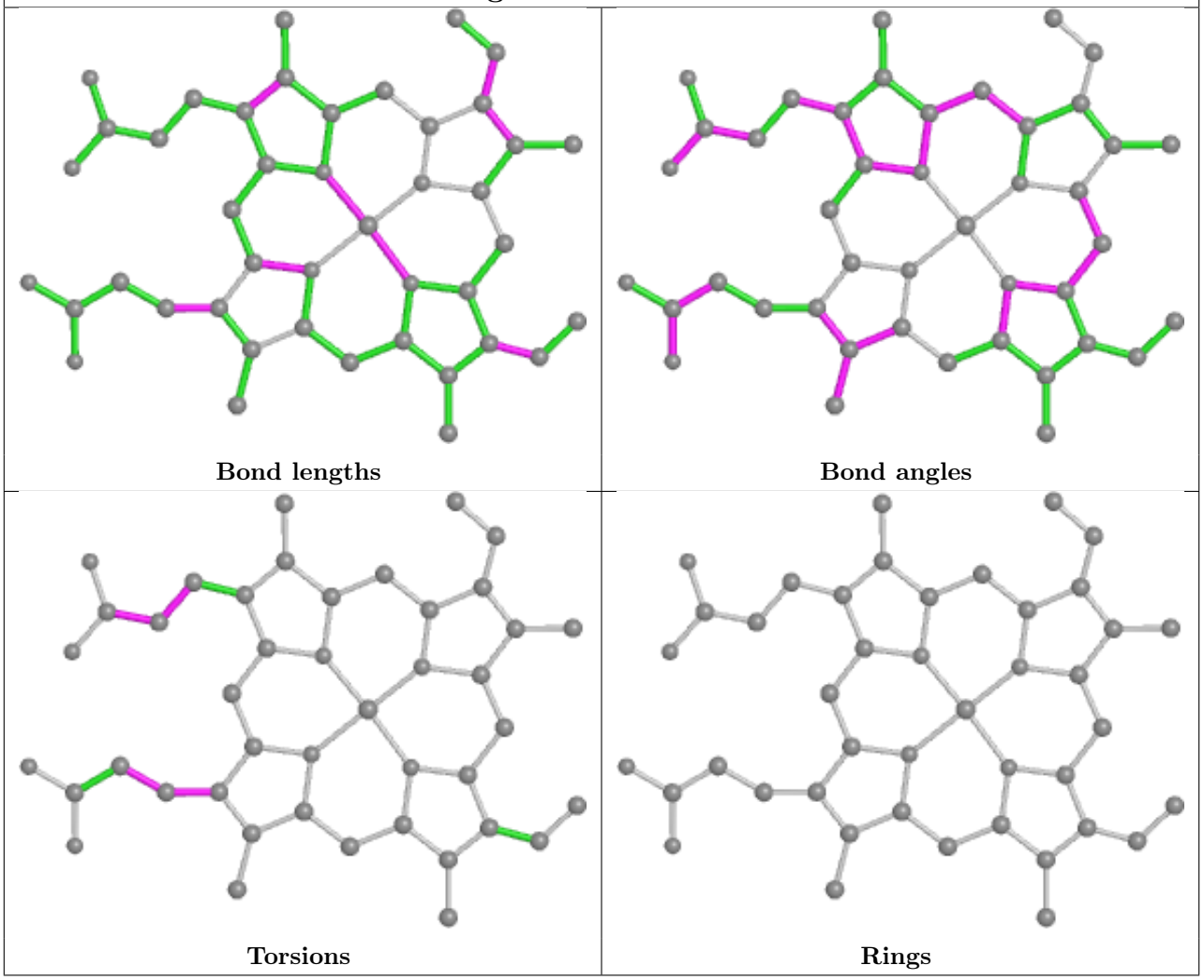


Torsions



Rings

Ligand HEM B 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	141/141 (100%)	-0.14	0 100 100	37, 56, 86, 124	0
1	D	141/141 (100%)	-0.10	0 100 100	40, 57, 84, 103	0
1	G	141/141 (100%)	-0.07	0 100 100	41, 60, 96, 132	0
1	J	141/141 (100%)	1.02	32 (22%) 0 0	110, 156, 201, 300	0
2	B	146/146 (100%)	-0.16	0 100 100	40, 84, 129, 196	0
2	E	146/146 (100%)	0.19	7 (4%) 30 27	47, 93, 138, 233	0
2	H	146/146 (100%)	-0.10	2 (1%) 75 75	48, 85, 131, 204	0
2	K	146/146 (100%)	2.15	63 (43%) 0 0	127, 182, 250, 268	0
3	C	309/347 (89%)	0.11	8 (2%) 56 52	45, 81, 121, 186	0
3	F	309/347 (89%)	0.13	7 (2%) 60 58	42, 72, 118, 165	1 (0%)
3	I	309/347 (89%)	-0.03	0 100 100	45, 67, 106, 133	0
3	L	309/347 (89%)	0.18	11 (3%) 42 37	66, 103, 141, 187	1 (0%)
All	All	2384/2536 (94%)	0.22	130 (5%) 25 21	37, 81, 176, 300	2 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	75	LEU	8.3
2	K	11	VAL	8.0
2	K	45	PHE	7.3
2	K	146	HIS	6.9
2	K	1	VAL	6.8
1	J	109	LEU	6.6
2	K	74	GLY	6.6
2	K	68	LEU	6.5
2	K	15	TRP	6.4
2	K	3	LEU	6.3
2	K	76	LYS	6.0

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Mol	Chain	Res	Type	RSRZ
2	K	71	PHE	5.9
1	J	30	GLU	5.9
2	K	81	LEU	5.8
1	J	117	PHE	5.5
2	E	146	HIS	5.5
2	K	143	HIS	5.5
2	K	67	VAL	5.4
2	K	9	GLU	5.3
2	K	18	VAL	5.1
3	L	151	ASN	5.0
2	K	4	SER	4.9
2	K	145	TYR	4.7
2	K	85	PHE	4.6
2	K	65	LYS	4.6
2	K	7	GLU	4.5
2	K	96	LEU	4.5
2	K	88	LEU	4.3
1	J	121	VAL	4.3
2	K	63	HIS	4.2
2	K	142	ALA	4.2
2	H	1	VAL	4.2
1	J	86	LEU	4.1
3	L	152	ASP	4.1
3	L	153	THR	4.0
1	J	110	ALA	4.0
2	K	13	GLY	4.0
2	K	2	HIS	3.9
3	C	51	HIS	3.8
2	K	78	LEU	3.8
1	J	56	LYS	3.8
2	K	72	SER	3.7
2	K	69	GLN	3.5
2	K	20	VAL	3.5
2	K	5	ALA	3.3
2	K	91	LEU	3.3
2	K	10	ALA	3.3
1	J	49	SER	3.3
2	K	120	HIS	3.3
1	J	43	PHE	3.3
3	L	154	LYS	3.2
1	J	79	ALA	3.2
2	K	6	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	45	HIS	3.2
2	K	141	LEU	3.2
1	J	88	ALA	3.1
2	K	60	VAL	3.1
1	J	53	ASP	3.1
3	F	50	TYR	3.0
2	K	130	PHE	3.0
1	J	141	ARG	3.0
2	K	79	ASP	3.0
2	E	144	LYS	3.0
3	L	150	LYS	2.9
1	J	10	VAL	2.9
1	J	111	ALA	2.8
2	E	12	LEU	2.8
2	K	122	PHE	2.8
1	J	32	MET	2.8
2	K	97	HIS	2.8
3	C	43	TYR	2.8
1	J	50	HIS	2.8
3	L	324	THR	2.7
2	K	80	ASN	2.7
2	K	82	LYS	2.7
2	K	58	PRO	2.6
2	H	2	HIS	2.6
3	L	179	PHE	2.6
2	K	14	LEU	2.6
2	K	16	GLY	2.6
2	K	73	ASP	2.6
2	K	19	ASN	2.6
3	L	326	GLU	2.6
1	J	84	SER	2.5
2	K	144	LYS	2.5
3	C	50	TYR	2.5
2	K	134	VAL	2.5
1	J	125	LEU	2.5
3	F	51	HIS	2.4
1	J	16	LYS	2.4
1	J	90	LYS	2.4
1	J	28	ALA	2.4
2	K	84	THR	2.3
3	C	46	HIS	2.3
3	L	66	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	68	LEU	2.3
1	J	108	THR	2.3
2	K	17	LYS	2.3
3	F	58	LEU	2.3
1	J	51	GLY	2.3
3	F	48	VAL	2.3
2	K	86	ALA	2.3
3	F	44	VAL	2.2
1	J	85	ASP	2.2
2	K	41	PHE	2.2
2	K	103	PHE	2.2
2	K	77	HIS	2.2
2	K	93	CYS	2.2
3	L	323	ARG	2.2
1	J	128	PHE	2.1
2	E	81	LEU	2.1
1	J	58	HIS	2.1
2	E	8	LYS	2.1
3	C	39	ILE	2.1
2	K	92	HIS	2.1
3	C	44	VAL	2.1
2	E	75	LEU	2.1
3	C	34	PRO	2.1
1	J	62	VAL	2.1
3	L	149	HIS	2.1
2	K	98	VAL	2.1
3	C	45	GLU	2.1
1	J	54	GLN	2.0
2	K	24	GLY	2.0
1	J	105	LEU	2.0
2	K	123	ASN	2.0
3	F	49	ARG	2.0
1	J	126	ASP	2.0
2	E	77	HIS	2.0
2	K	8	LYS	2.0

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

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

6.3 Carbohydrates (i)

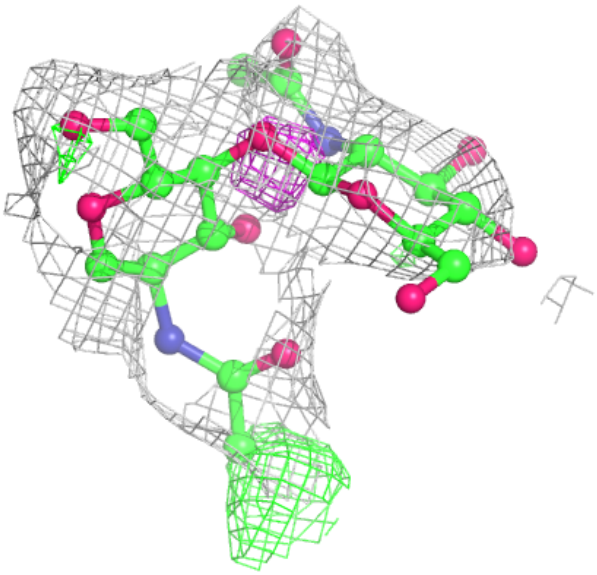
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

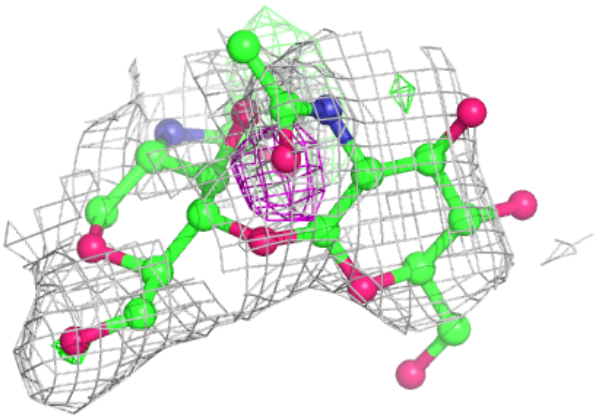
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	Q	1	14/15	0.72	0.19	126,126,126,126	0
5	FUC	P	2	10/11	0.72	0.46	149,149,149,149	0
4	NAG	O	1	14/15	0.74	0.20	118,118,118,118	0
5	NAG	N	1	14/15	0.77	0.37	138,138,138,138	0
5	NAG	S	1	14/15	0.77	0.28	212,212,212,212	0
5	NAG	P	1	14/15	0.79	0.42	135,135,135,135	0
4	NAG	M	1	14/15	0.79	0.16	122,122,122,122	0
4	NAG	O	2	14/15	0.79	0.25	161,161,161,161	0
4	NAG	M	2	14/15	0.80	0.34	180,180,180,180	0
5	NAG	R	1	14/15	0.82	0.35	141,141,141,141	0
5	FUC	S	2	10/11	0.82	0.28	188,188,188,188	0
4	NAG	Q	2	14/15	0.84	0.32	168,168,168,168	0
5	FUC	R	2	10/11	0.87	0.25	148,148,148,148	0
5	FUC	N	2	10/11	0.92	0.21	138,138,138,138	0

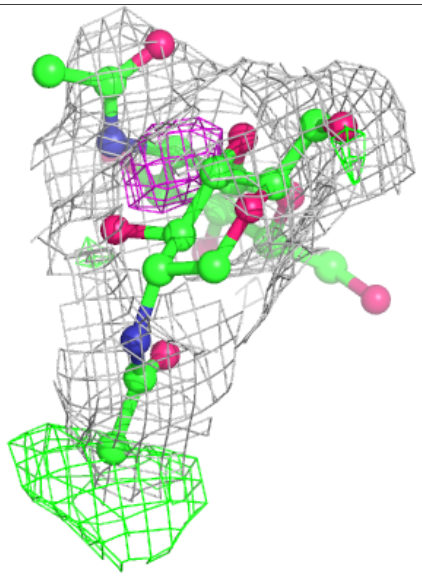
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

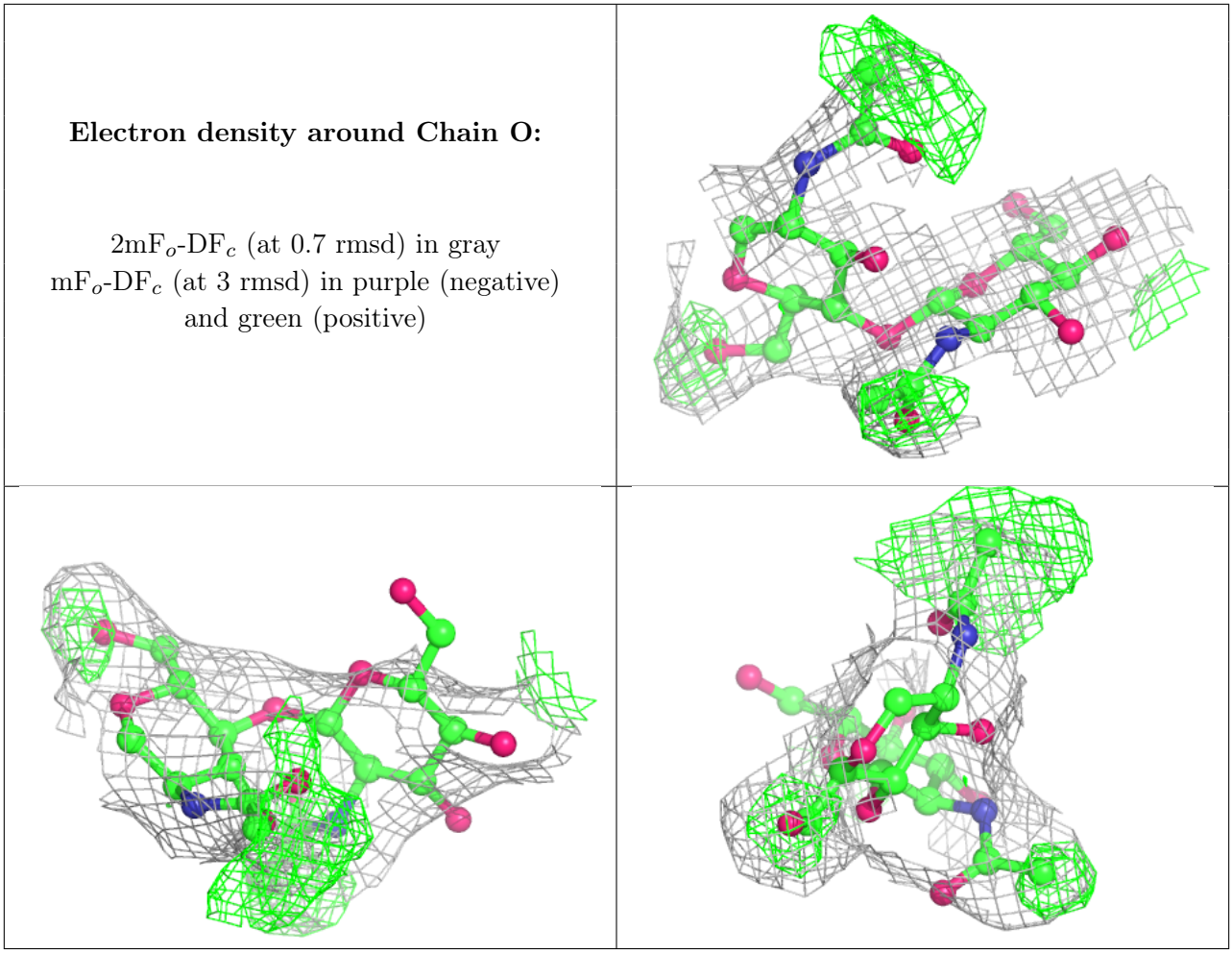






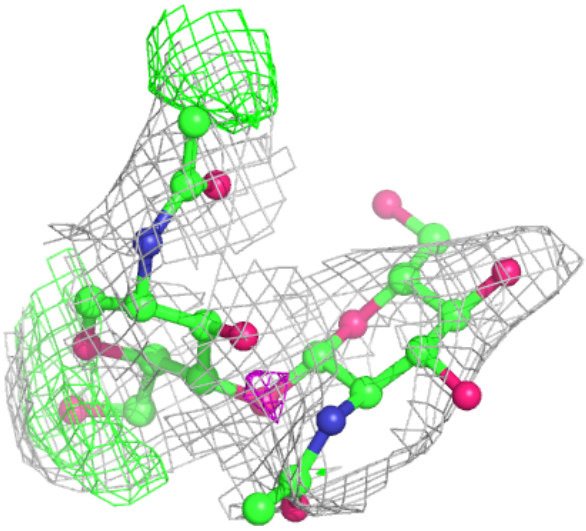
Electron density around Chain O:

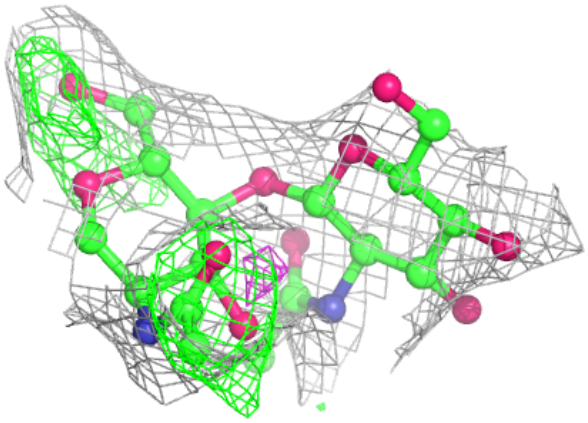
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

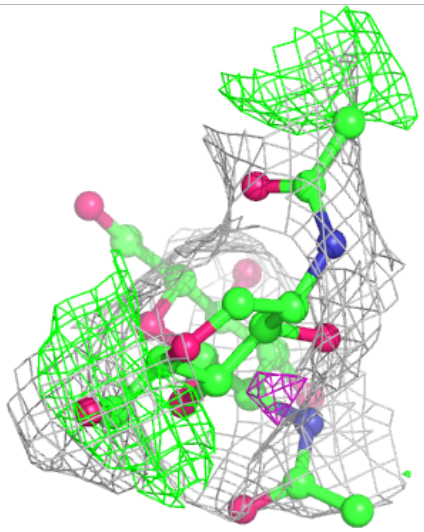


Electron density around Chain Q:

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

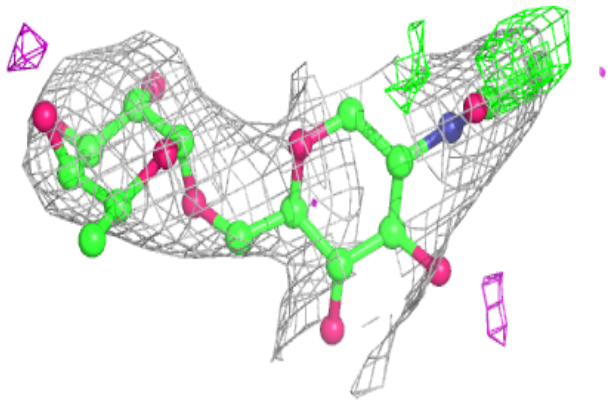


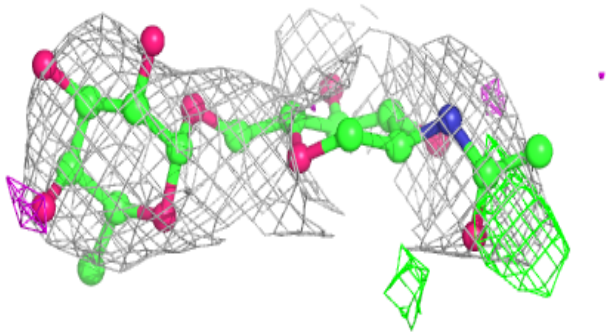


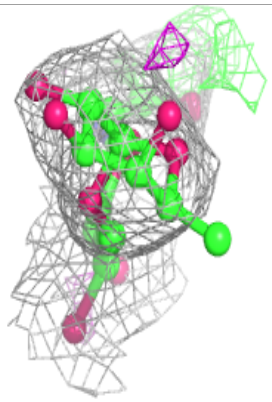


Electron density around Chain N:

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

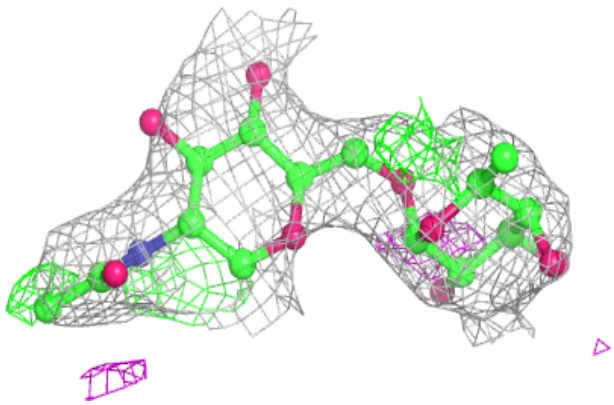


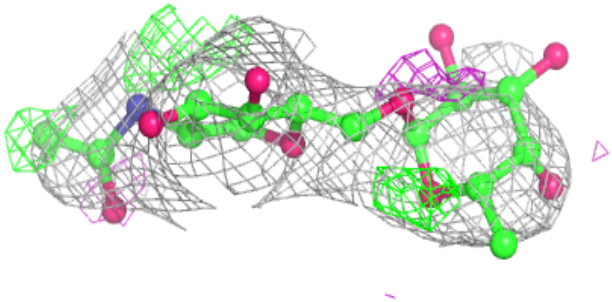


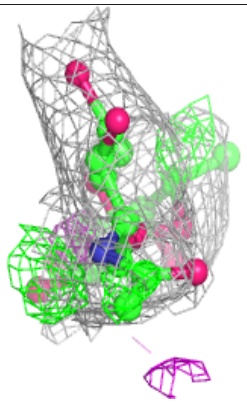


Electron density around Chain P:

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

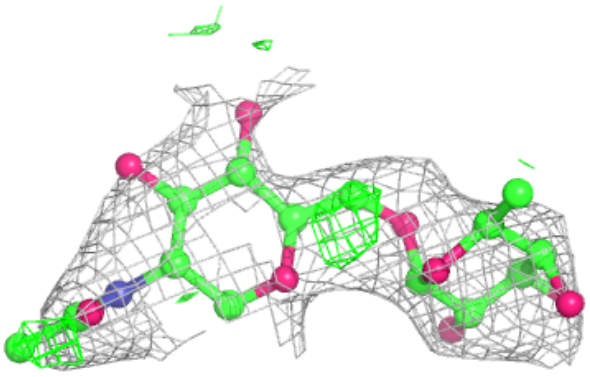


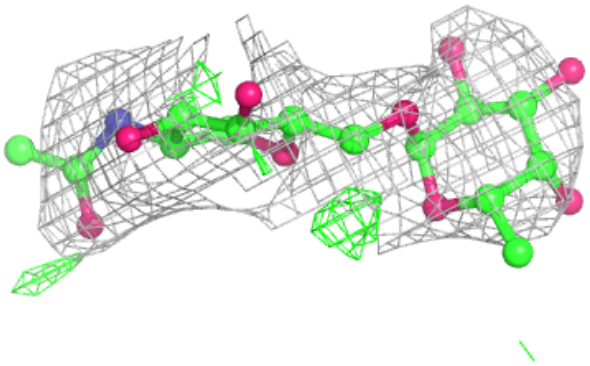


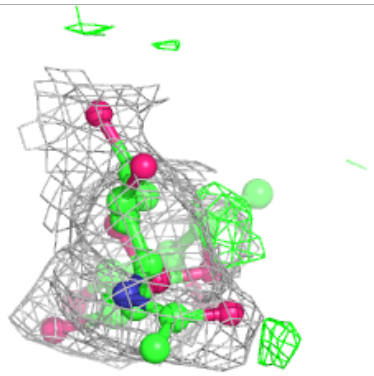


Electron density around Chain R:

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

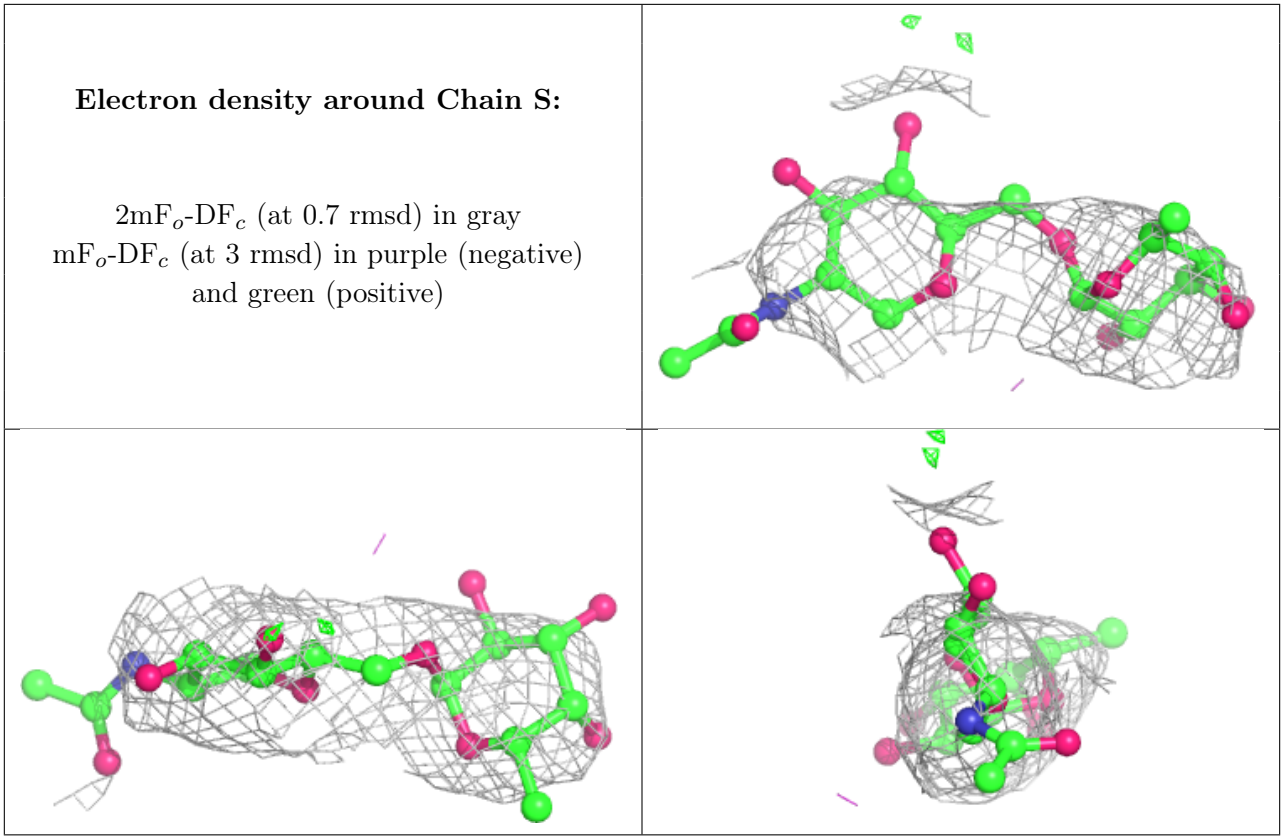






Electron density around Chain S:

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



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	C	1003	14/15	0.49	0.46	172,172,172,172	0
8	NAG	I	1004	14/15	0.64	0.29	150,150,150,150	0
8	NAG	I	1003	14/15	0.67	0.41	164,164,164,164	0
8	NAG	L	1001	14/15	0.71	0.17	138,138,138,138	0
8	NAG	F	1004	14/15	0.72	0.30	144,144,144,144	0
8	NAG	F	1003	14/15	0.72	0.53	174,174,174,174	0
8	NAG	L	1002	14/15	0.81	0.29	171,171,171,171	0
8	NAG	C	1004	14/15	0.84	0.25	159,159,159,159	0
6	HEM	J	201	43/43	0.93	0.34	183,186,190,191	0
6	HEM	K	201	43/43	0.93	0.32	167,186,195,199	0
6	HEM	E	201	43/43	0.96	0.23	95,101,114,121	0
7	OXY	J	202	2/2	0.97	0.21	225,225,225,229	0
6	HEM	B	201	43/43	0.97	0.21	76,80,95,103	0
6	HEM	H	201	43/43	0.97	0.25	83,87,101,109	0

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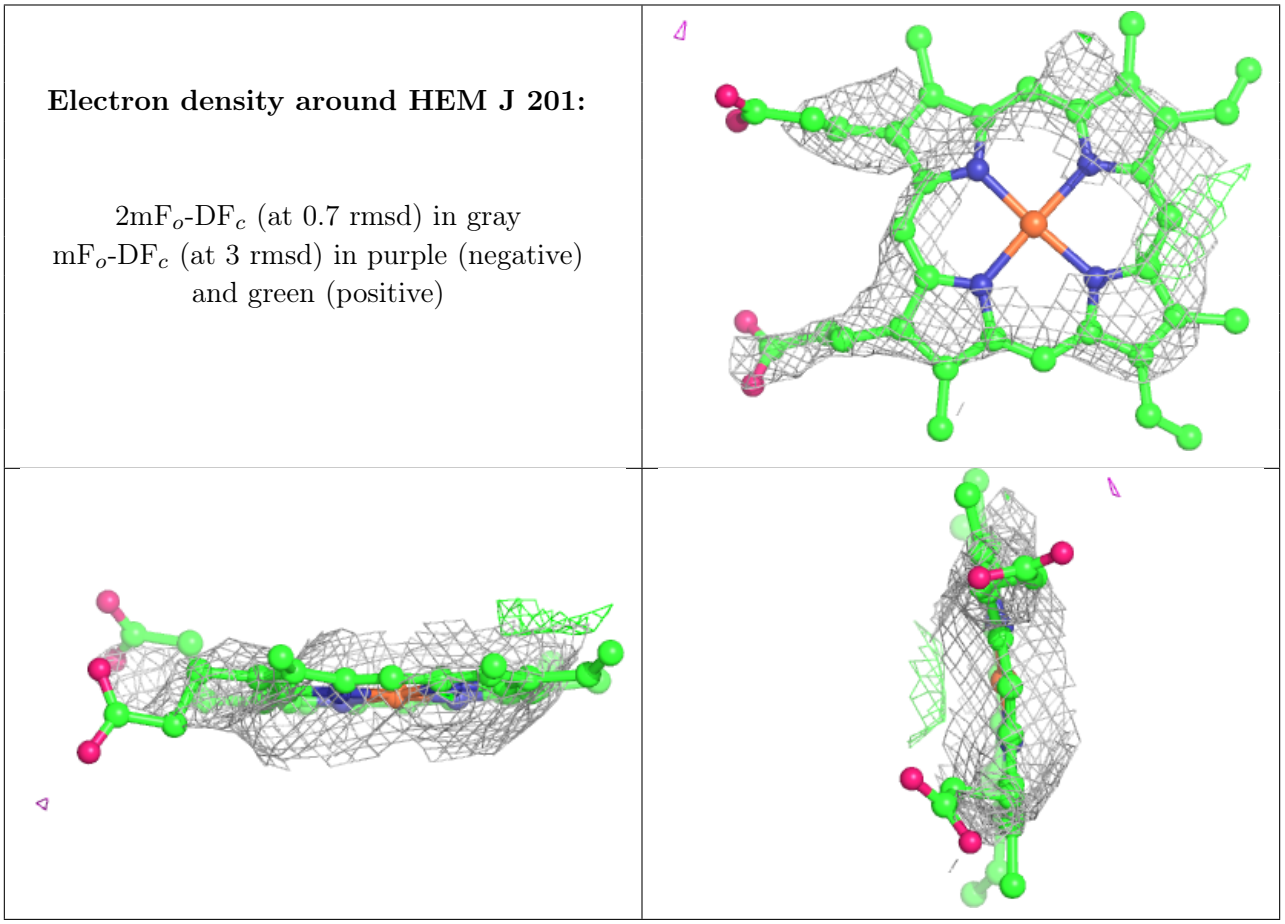
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	OXY	K	202	2/2	0.98	0.47	292,292,292,295	0
6	HEM	D	201	43/43	0.98	0.19	45,51,57,59	0
6	HEM	G	201	43/43	0.98	0.19	41,58,62,64	0
6	HEM	A	201	43/43	0.99	0.18	45,54,62,63	0
7	OXY	A	202	2/2	0.99	0.38	92,92,92,96	0
7	OXY	E	202	2/2	0.99	0.16	146,146,146,148	0
7	OXY	G	202	2/2	0.99	0.49	101,101,101,105	0
7	OXY	H	202	2/2	0.99	0.24	174,174,174,176	0
7	OXY	D	202	2/2	1.00	0.22	84,84,84,88	0
7	OXY	B	202	2/2	1.00	0.18	121,121,121,123	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.

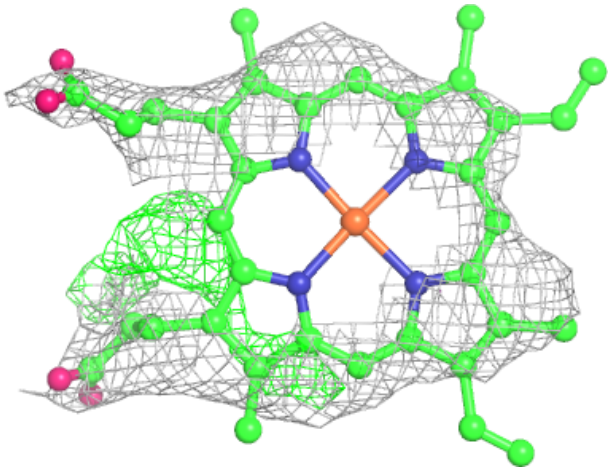
Electron density around HEM J 201:

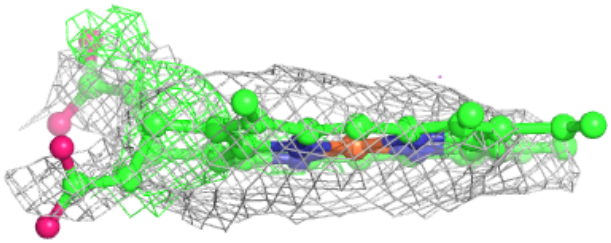
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

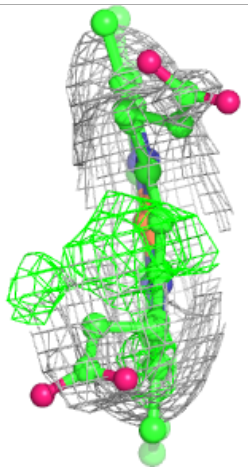


Electron density around HEM K 201:

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

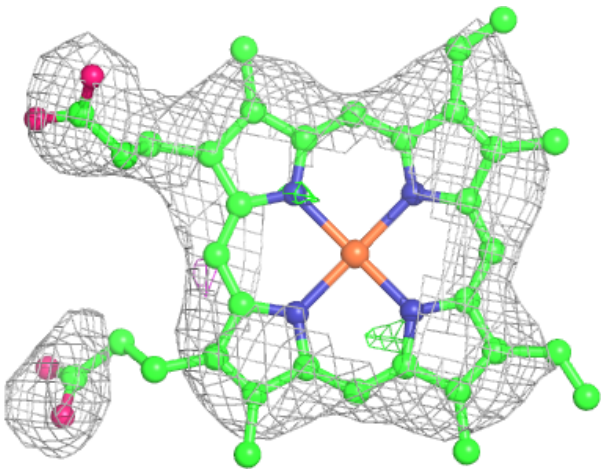


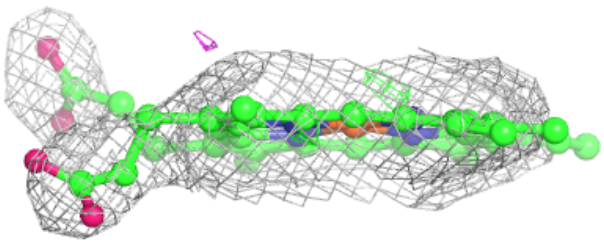


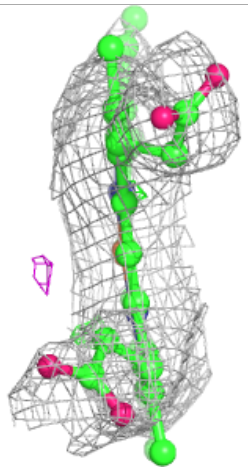


Electron density around HEM E 201:

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

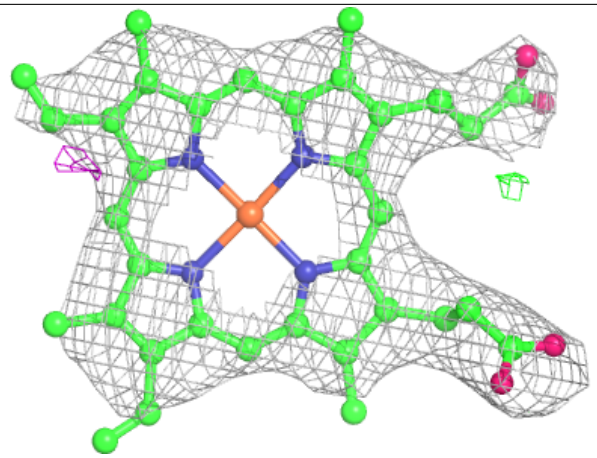


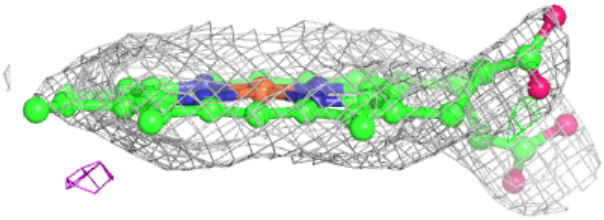


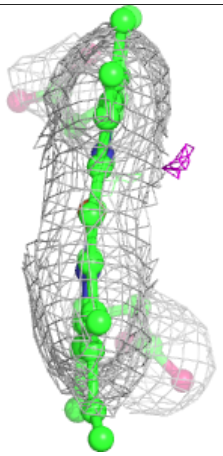


Electron density around HEM B 201:

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

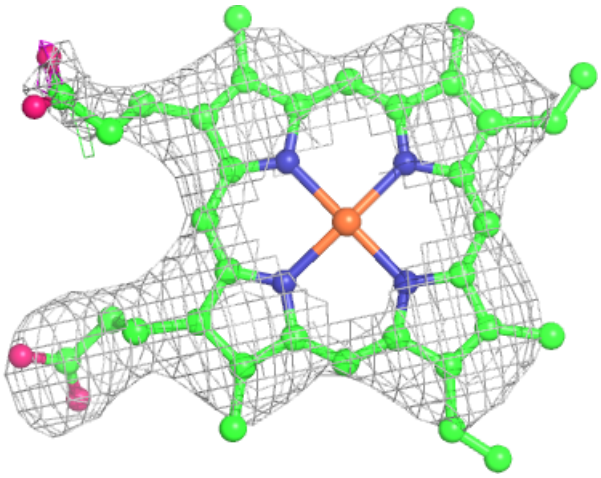


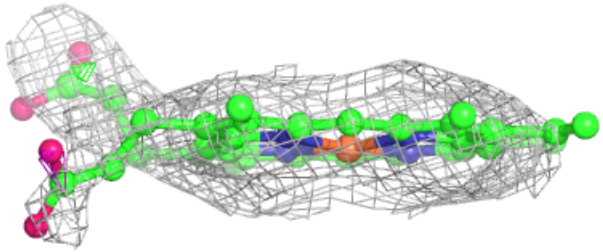


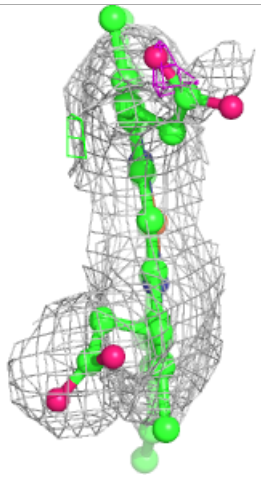


Electron density around HEM H 201:

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

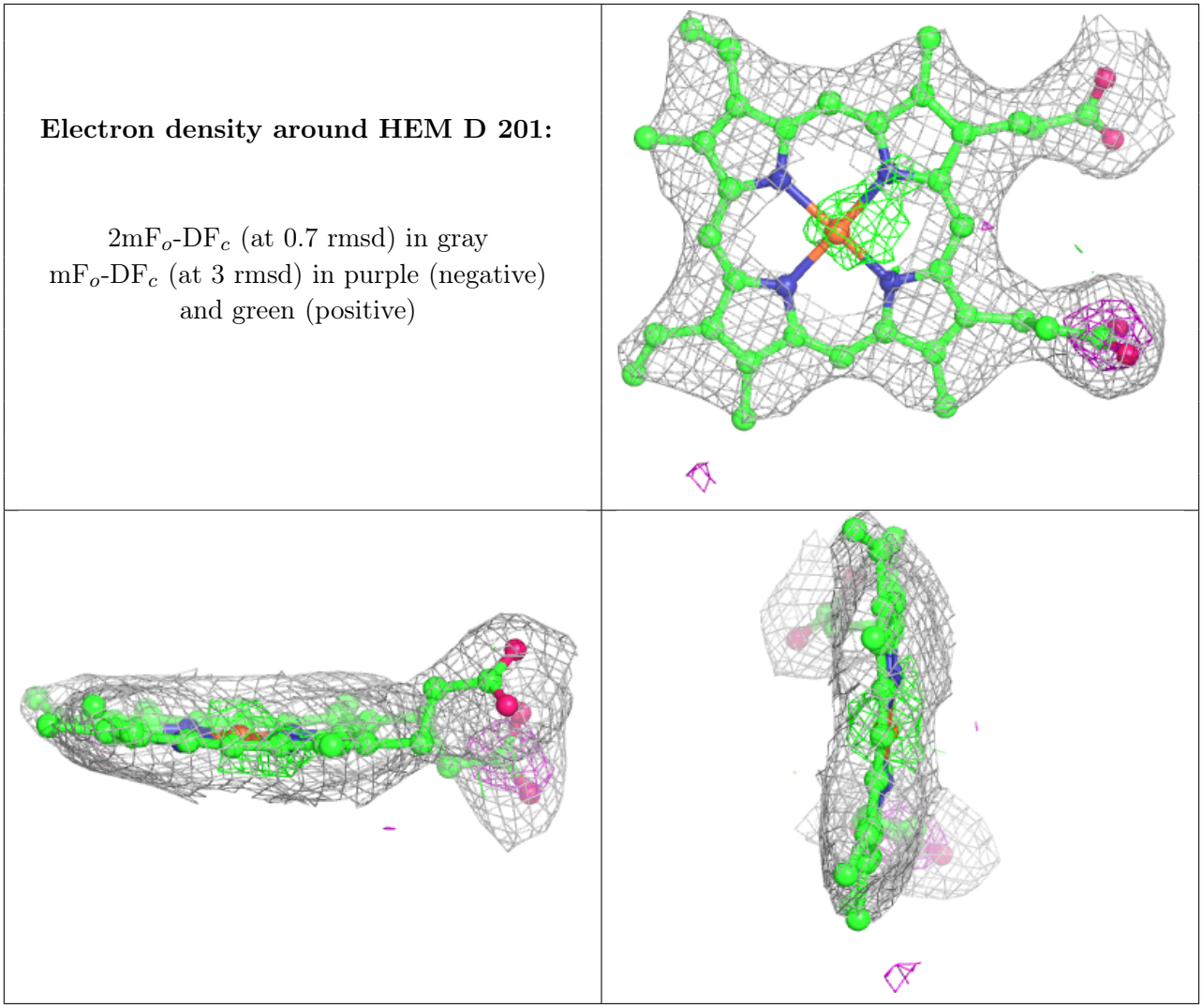






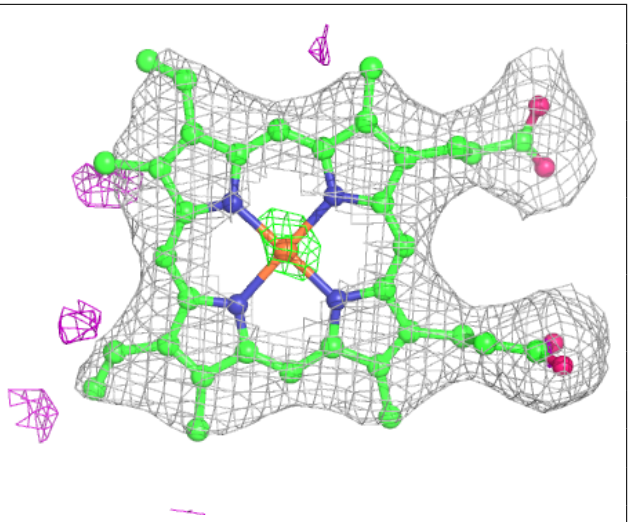
Electron density around HEM D 201:

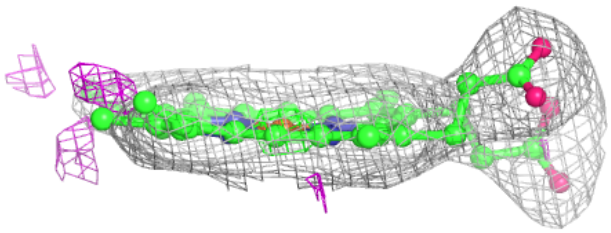
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

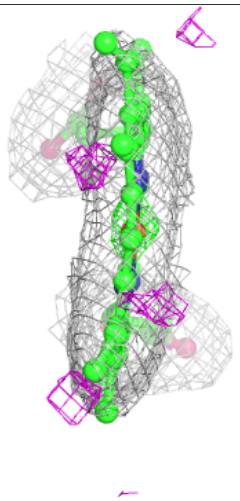


Electron density around HEM G 201:

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

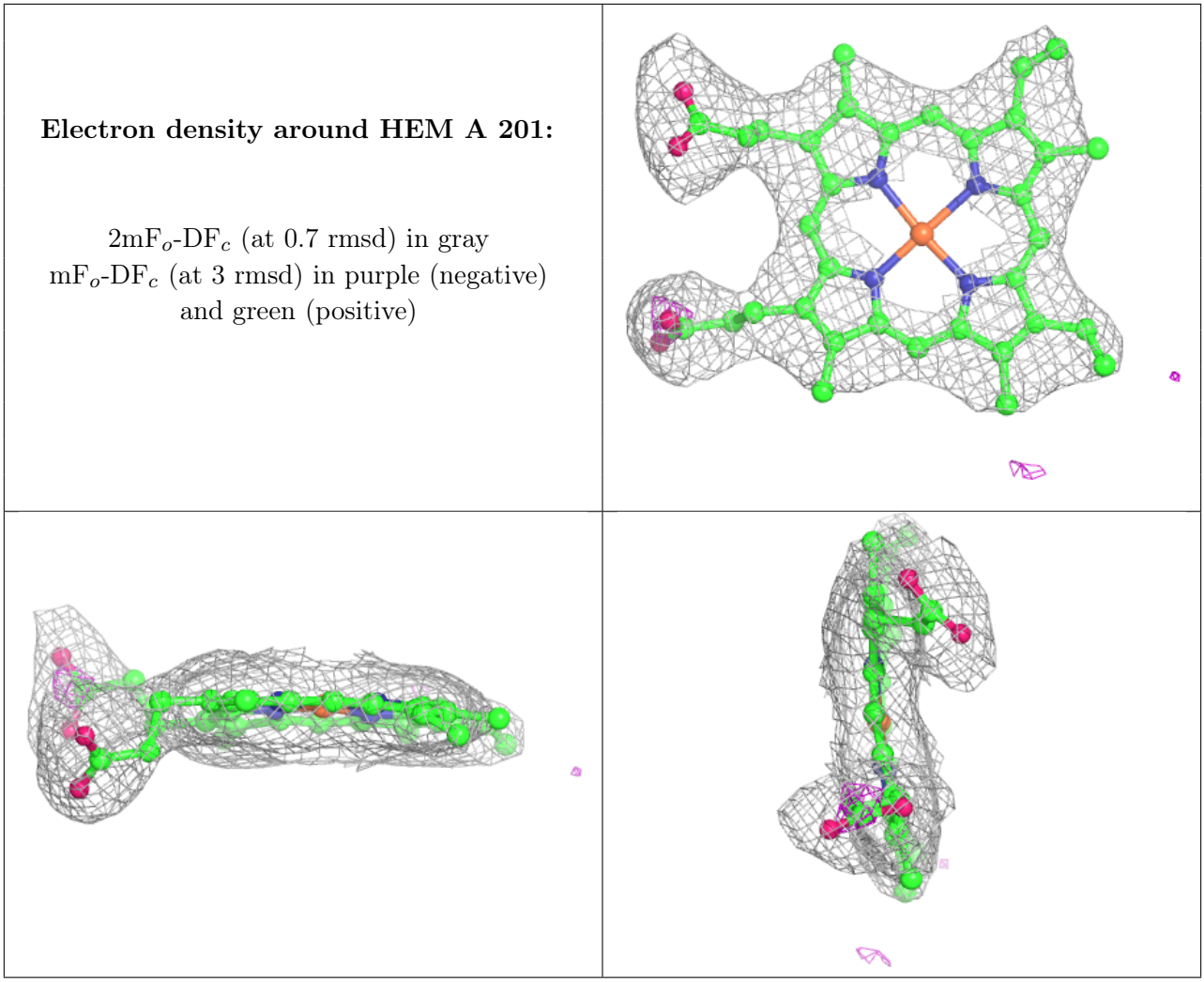






Electron density around HEM A 201:

$2mF_o$-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.