Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 04:49 AM EDT

PDB ID	:	4WJG
Title	:	Structure of T. brucei haptoglobin-hemoglobin receptor binding to human haptoglobin-hemoglobin
Authors	:	Stoedkilde, K.; Torvund-Jensen, M.; Moestrup, S.K.; Andersen, C.B.F.
Deposited on	:	2014-09-30
Resolution	:	3.10 Å(reported)

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

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

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

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

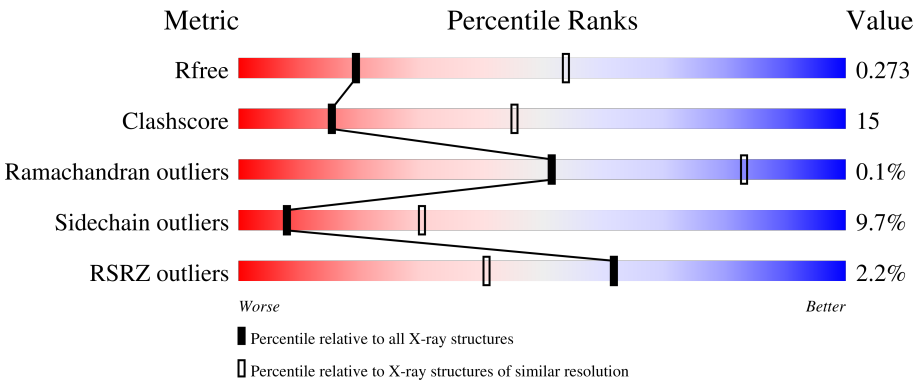
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	67% 28% •
1	F	141	70% 26% •
1	K	141	68% 28% •
1	P	141	70% 27% •
1	U	141	67% 29% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Z	141	67% 30% •
2	1	146	% 68% 29% •
2	B	146	65% 33% •
2	G	146	% 66% 31% •
2	L	146	63% 34% •
2	Q	146	62% 36% •
2	V	146	67% 29% •
3	2	315	59% 35% • •
3	C	315	57% 36% 6% •
3	H	315	% 57% 36% 5% •
3	M	315	57% 37% 5% •
3	R	315	57% 36% 5% •
3	W	315	% 58% 34% 6% •
4	3	146	% 75% 22% ••
4	D	146	% 75% 22% ••
4	I	146	74% 23% ••
4	N	146	% 75% 23% ••
4	S	146	73% 25% ••
4	X	146	% 75% 22% ••
5	4	343	5% 51% 20% • 24%
5	E	343	4% 52% 19% 5% 24%
5	J	343	7% 51% 21% • 24%
5	O	343	4% 51% 20% • 24%
5	T	343	7% 50% 21% • 24%
5	Y	343	7% 51% 21% • 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	a	2	100%
6	b	2	50% 50%
6	c	2	100%
6	d	2	100%
6	e	2	100%
6	f	2	100%
6	g	2	100%
6	h	2	100%
6	i	2	100%
6	j	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
9	NAG	C	1001	-	-	-	X
9	NAG	C	1004	-	-	-	X
9	NAG	J	1001	-	-	-	X
9	NAG	M	1004	-	-	-	X
9	NAG	R	1004	-	-	-	X
9	NAG	T	1001	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 47792 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
			Total	C	N	O	S			
1	A	141	1069	685	187	194	3	0	0	0
1	F	141	1069	685	187	194	3	0	0	0
1	K	141	1069	685	187	194	3	0	0	0
1	P	141	1069	685	187	194	3	0	0	0
1	U	141	1069	685	187	194	3	0	0	0
1	Z	141	1069	685	187	194	3	0	0	0

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	146	1123	724	195	201	3	0	0	0
2	G	146	1123	724	195	201	3	0	0	0
2	L	146	1123	724	195	201	3	0	0	0
2	Q	146	1123	724	195	201	3	0	0	0
2	V	146	1123	724	195	201	3	0	0	0
2	1	146	1123	724	195	201	3	0	0	0

- Molecule 3 is a protein called Haptoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	310	2437	1552	413	459	13	0	0	0
3	H	310	2437	1552	413	459	13	0	0	0
3	M	310	2437	1552	413	459	13	0	0	0
3	R	310	2437	1552	413	459	13	0	0	0
3	W	310	2437	1552	413	459	13	0	0	0
3	2	310	2437	1552	413	459	13	0	0	0

- Molecule 4 is a protein called Iron-regulated surface determinant protein H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	144	1183	754	189	240	0	0	0
4	I	144	1183	754	189	240	0	0	0
4	N	144	1183	754	189	240	0	0	0
4	S	144	1183	754	189	240	0	0	0
4	X	144	1183	754	189	240	0	0	0
4	3	144	1183	754	189	240	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	84	GLY	-	expression tag	UNP Q99TD3
D	85	SER	-	expression tag	UNP Q99TD3
I	84	GLY	-	expression tag	UNP Q99TD3
I	85	SER	-	expression tag	UNP Q99TD3
N	84	GLY	-	expression tag	UNP Q99TD3
N	85	SER	-	expression tag	UNP Q99TD3
S	84	GLY	-	expression tag	UNP Q99TD3
S	85	SER	-	expression tag	UNP Q99TD3
X	84	GLY	-	expression tag	UNP Q99TD3
X	85	SER	-	expression tag	UNP Q99TD3
3	84	GLY	-	expression tag	UNP Q99TD3
3	85	SER	-	expression tag	UNP Q99TD3

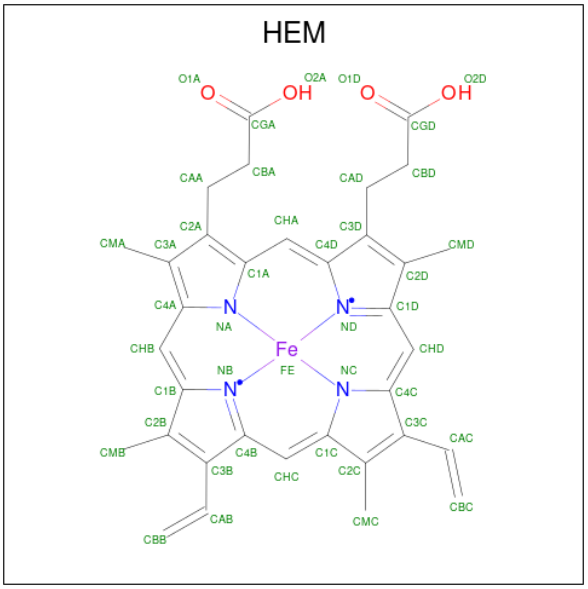
- Molecule 5 is a protein called Haptoglobin-hemoglobin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	261	1963	1202	365	393	3	0	0	0
5	J	261	1963	1202	365	393	3	0	0	0
5	O	261	1963	1202	365	393	3	0	0	0
5	T	261	1963	1202	365	393	3	0	0	0
5	Y	261	1963	1202	365	393	3	0	0	0
5	4	261	1963	1202	365	393	3	0	0	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

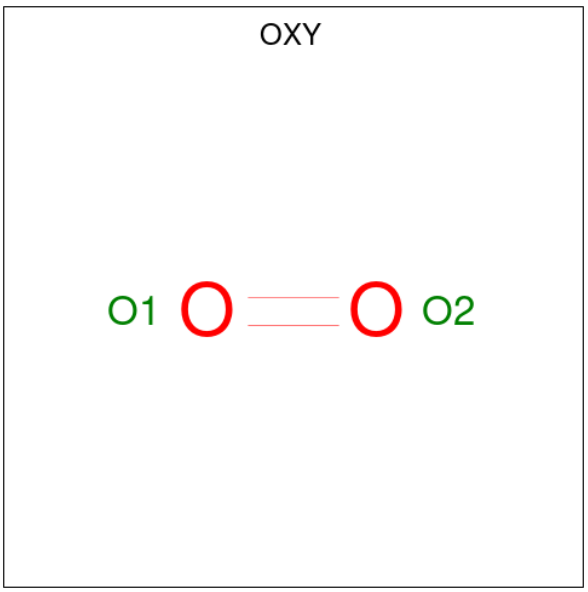
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	a	2	28	16	2	10	0	0	0
6	b	2	28	16	2	10	0	0	0
6	c	2	28	16	2	10	0	0	0
6	d	2	28	16	2	10	0	0	0
6	e	2	28	16	2	10	0	0	0
6	f	2	28	16	2	10	0	0	0
6	g	2	28	16	2	10	0	0	0
6	h	2	28	16	2	10	0	0	0
6	i	2	28	16	2	10	0	0	0
6	j	2	28	16	2	10	0	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
7	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	G	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	K	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	L	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	P	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	Q	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	U	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	V	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	Z	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	1	1	43	34	1	4	4	0	0

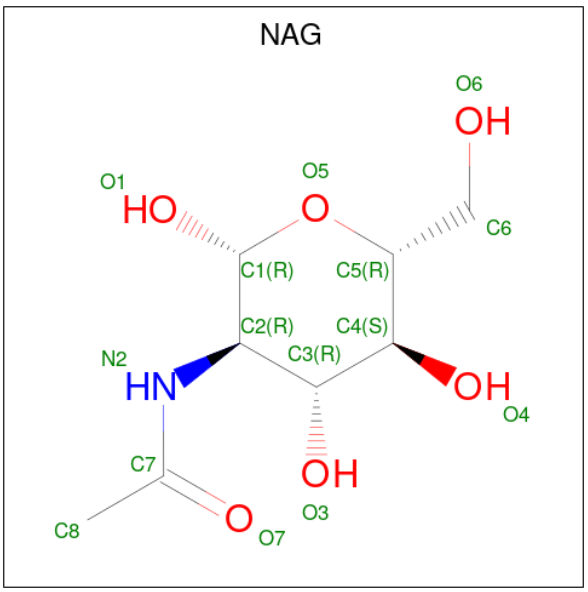
- Molecule 8 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0
8	F	1	Total O 2 2	0	0
8	G	1	Total O 2 2	0	0
8	K	1	Total O 2 2	0	0
8	L	1	Total O 2 2	0	0
8	P	1	Total O 2 2	0	0
8	Q	1	Total O 2 2	0	0
8	U	1	Total O 2 2	0	0
8	V	1	Total O 2 2	0	0
8	Z	1	Total O 2 2	0	0
8	1	1	Total O 2 2	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	C	1	14	8	1	5	0	0
			Total	C	N	O		
9	C	1	14	8	1	5	0	0
			Total	C	N	O		
9	E	1	14	8	1	5	0	0
			Total	C	N	O		
9	E	1	14	8	1	5	0	0
			Total	C	N	O		
9	H	1	14	8	1	5	0	0
			Total	C	N	O		
9	H	1	14	8	1	5	0	0
			Total	C	N	O		
9	J	1	14	8	1	5	0	0
			Total	C	N	O		
9	J	1	14	8	1	5	0	0
			Total	C	N	O		
9	M	1	14	8	1	5	0	0
			Total	C	N	O		
9	M	1	14	8	1	5	0	0
			Total	C	N	O		
9	O	1	14	8	1	5	0	0
			Total	C	N	O		
9	O	1	14	8	1	5	0	0
			Total	C	N	O		
9	R	1	14	8	1	5	0	0

Continued on next page...

Continued from previous page...

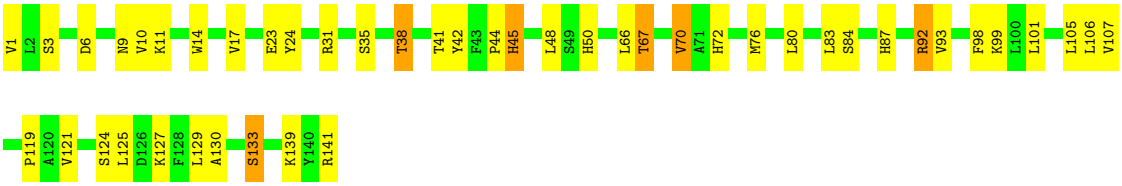
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	R	1	14	8	1	5	0	0
			Total	C	N	O		
9	T	1	14	8	1	5	0	0
			Total	C	N	O		
9	T	1	14	8	1	5	0	0
			Total	C	N	O		
9	W	1	14	8	1	5	0	0
			Total	C	N	O		
9	W	1	14	8	1	5	0	0
			Total	C	N	O		
9	Y	1	14	8	1	5	0	0
			Total	C	N	O		
9	Y	1	14	8	1	5	0	0
			Total	C	N	O		
9	2	1	14	8	1	5	0	0
			Total	C	N	O		
9	4	1	14	8	1	5	0	0
			Total	C	N	O		
9	4	1	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.

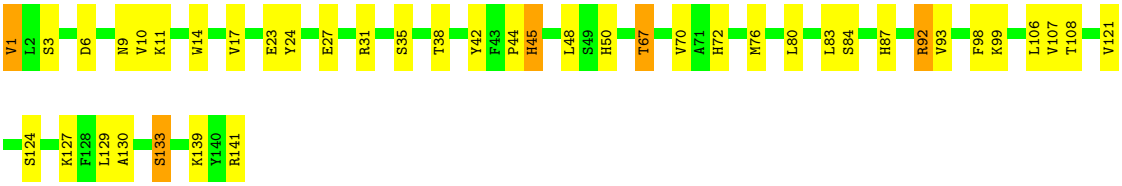
• Molecule 1: Hemoglobin subunit alpha

Chain A:



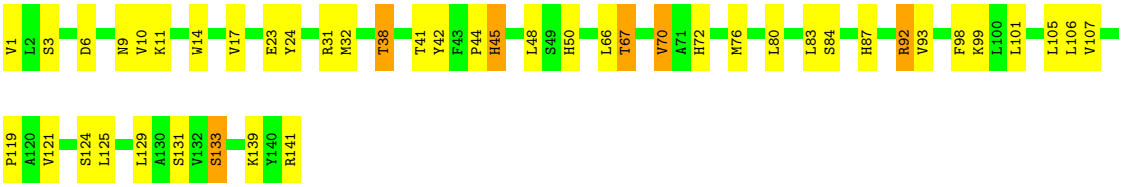
• Molecule 1: Hemoglobin subunit alpha

Chain F:



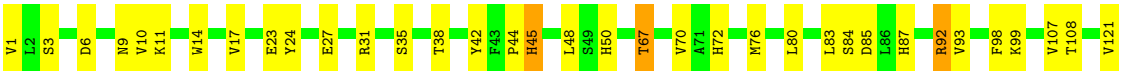
• Molecule 1: Hemoglobin subunit alpha

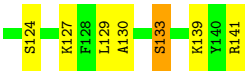
Chain K:



• Molecule 1: Hemoglobin subunit alpha

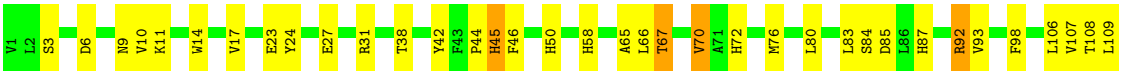
Chain P:

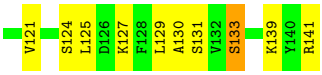




• Molecule 1: Hemoglobin subunit alpha

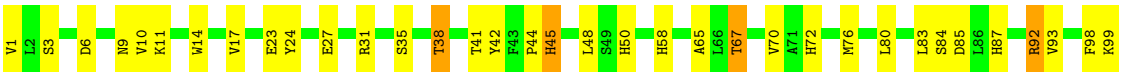
Chain U:

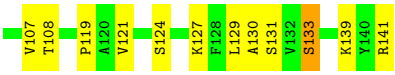




• Molecule 1: Hemoglobin subunit alpha

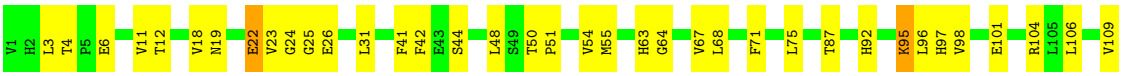
Chain Z:





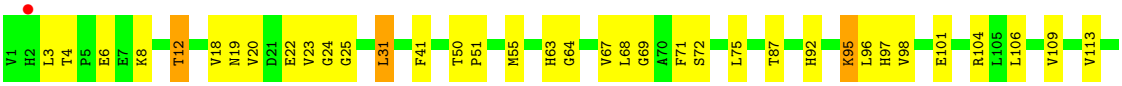
• Molecule 2: Hemoglobin subunit beta

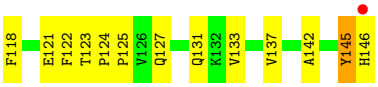
Chain B:



• Molecule 2: Hemoglobin subunit beta

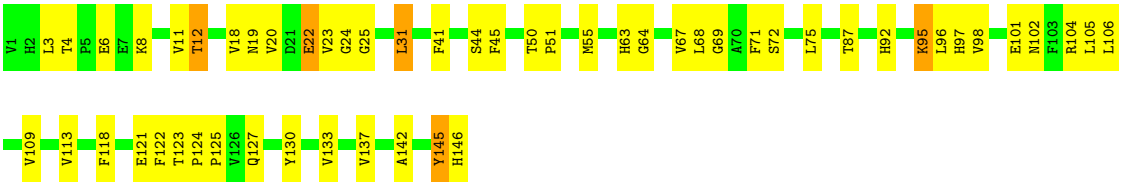
Chain G:





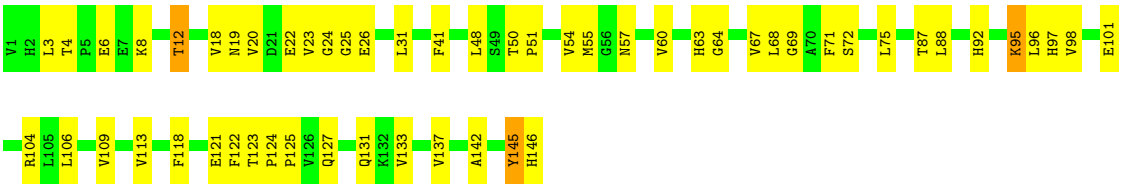
• Molecule 2: Hemoglobin subunit beta

Chain L:



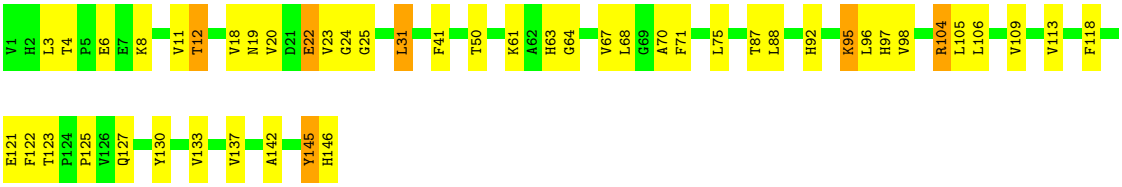
• Molecule 2: Hemoglobin subunit beta

Chain Q:



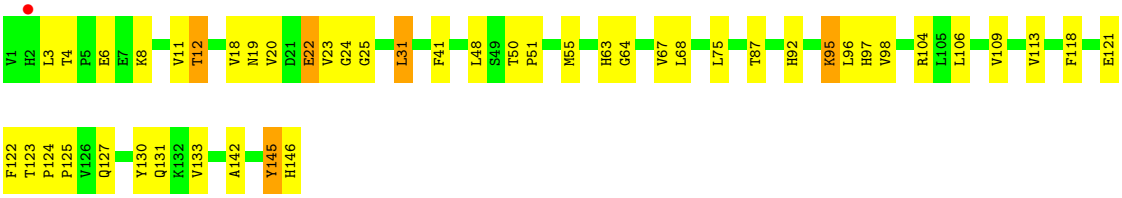
• Molecule 2: Hemoglobin subunit beta

Chain V:



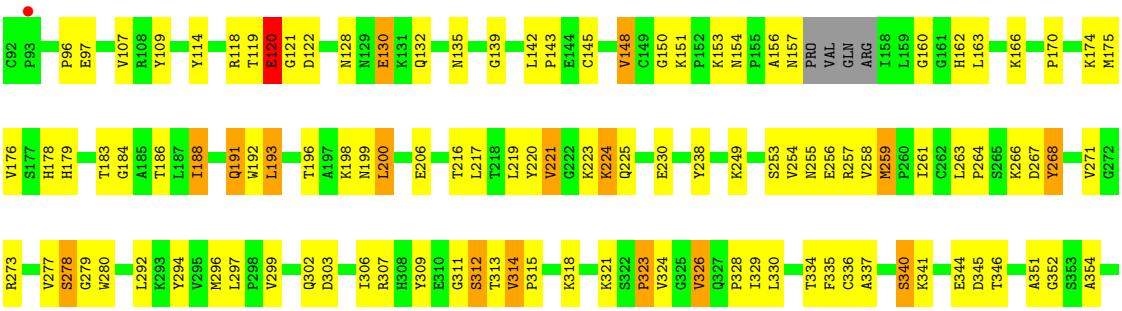
• Molecule 2: Hemoglobin subunit beta

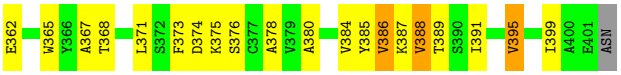
Chain 1:



• Molecule 3: Haptoglobin

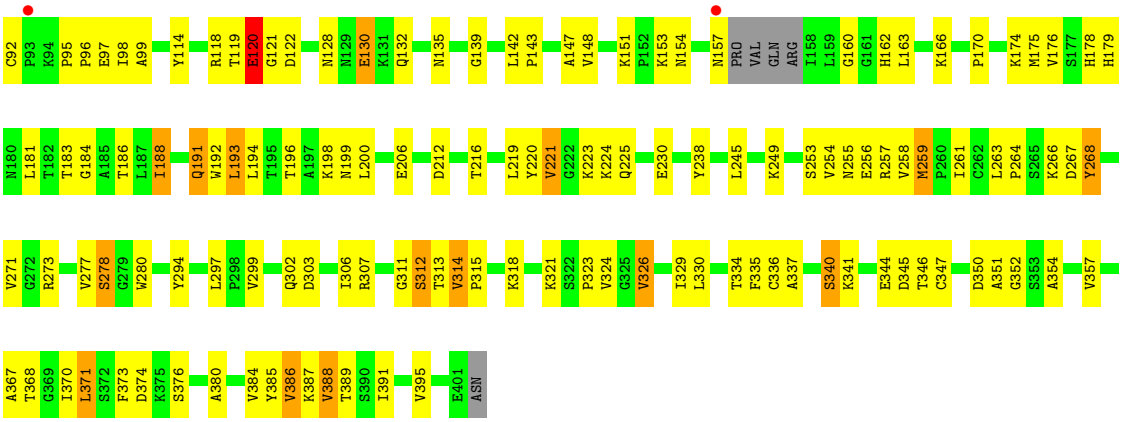
Chain C:





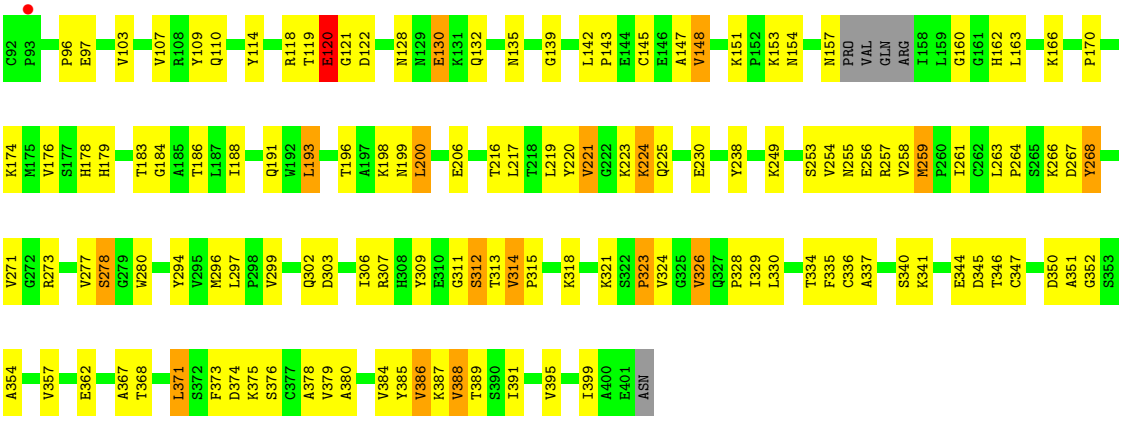
- Molecule 3: Haptoglobin

Chain H:



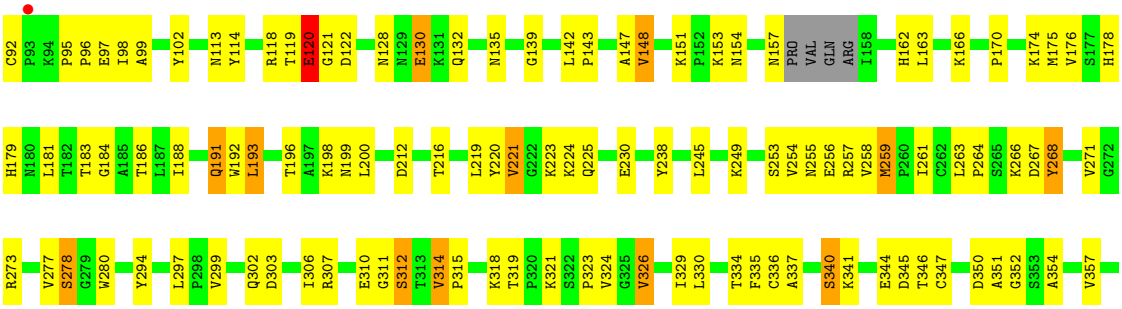
- Molecule 3: Haptoglobin

Chain M:



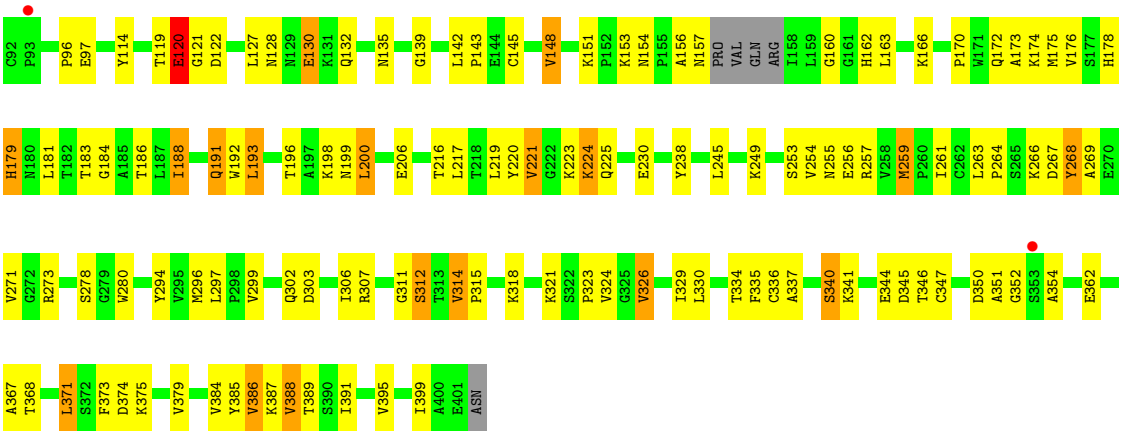
- Molecule 3: Haptoglobin

Chain R:



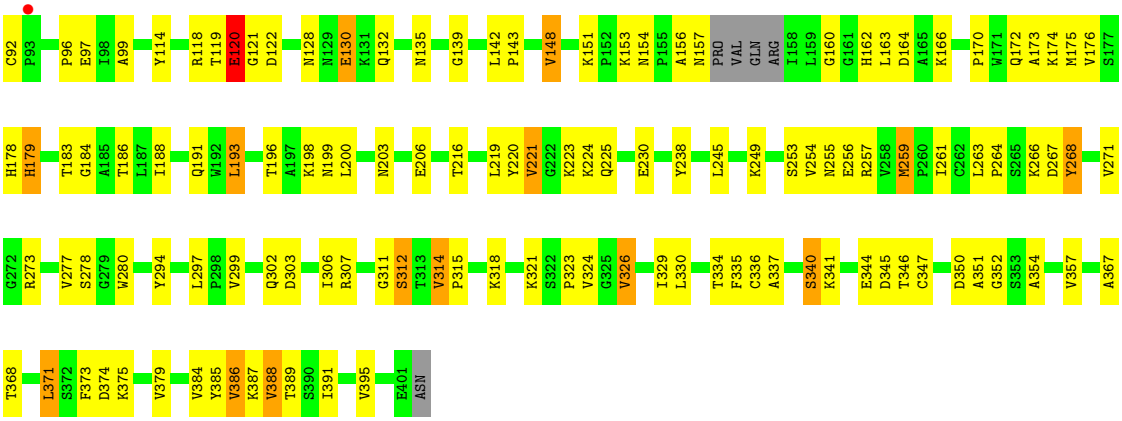
• Molecule 3: Haptoglobin

Chain W:



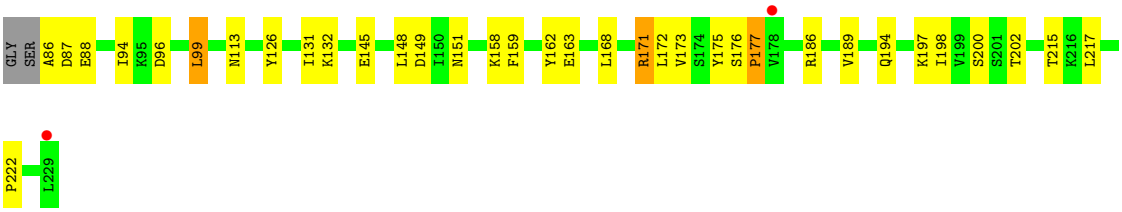
• Molecule 3: Haptoglobin

Chain 2:



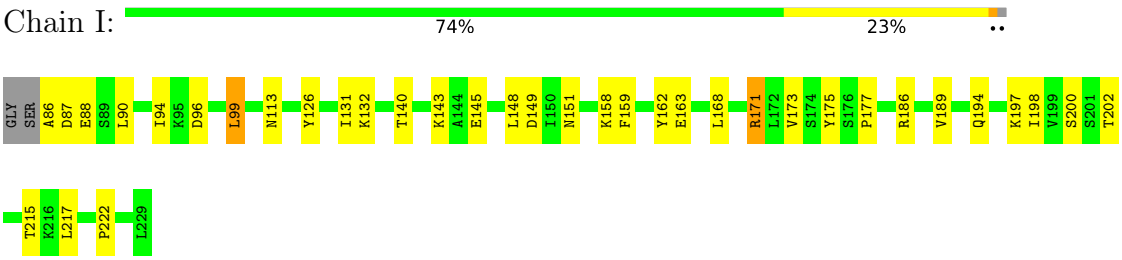
• Molecule 4: Iron-regulated surface determinant protein H

Chain D:



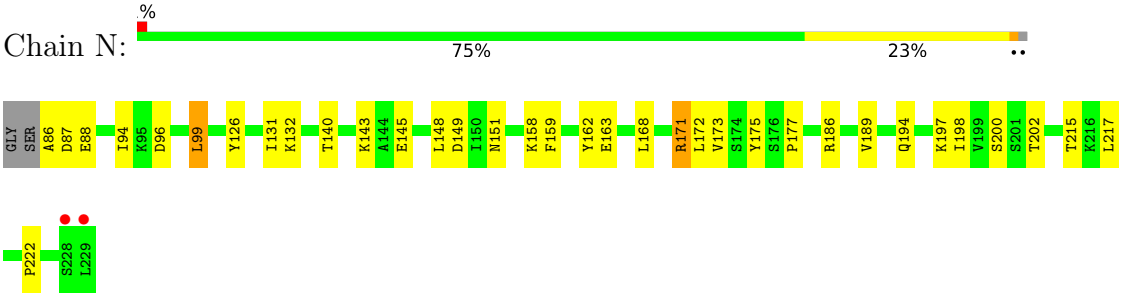
• Molecule 4: Iron-regulated surface determinant protein H

Chain I:



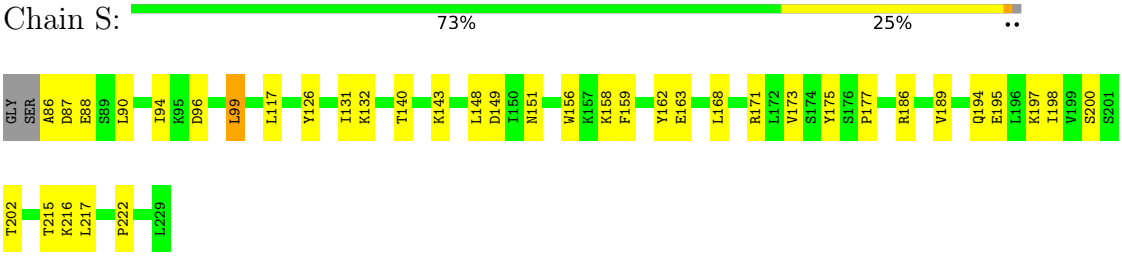
• Molecule 4: Iron-regulated surface determinant protein H

Chain N:



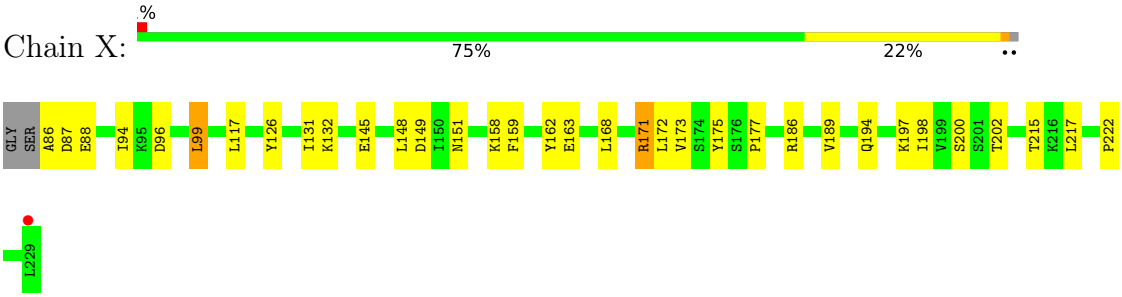
• Molecule 4: Iron-regulated surface determinant protein H

Chain S:



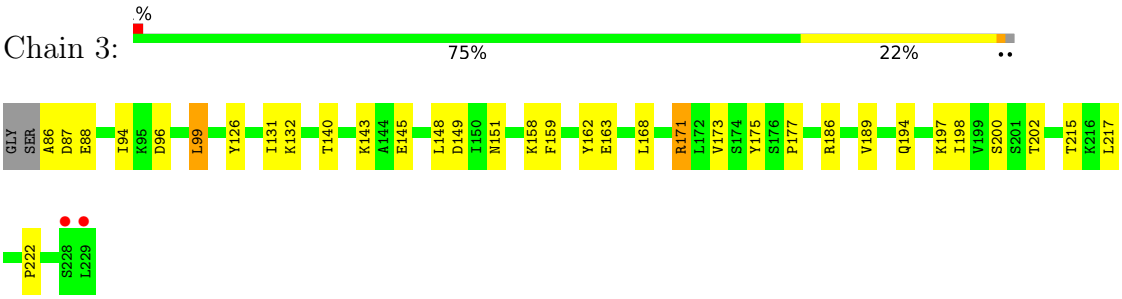
• Molecule 4: Iron-regulated surface determinant protein H

Chain X:



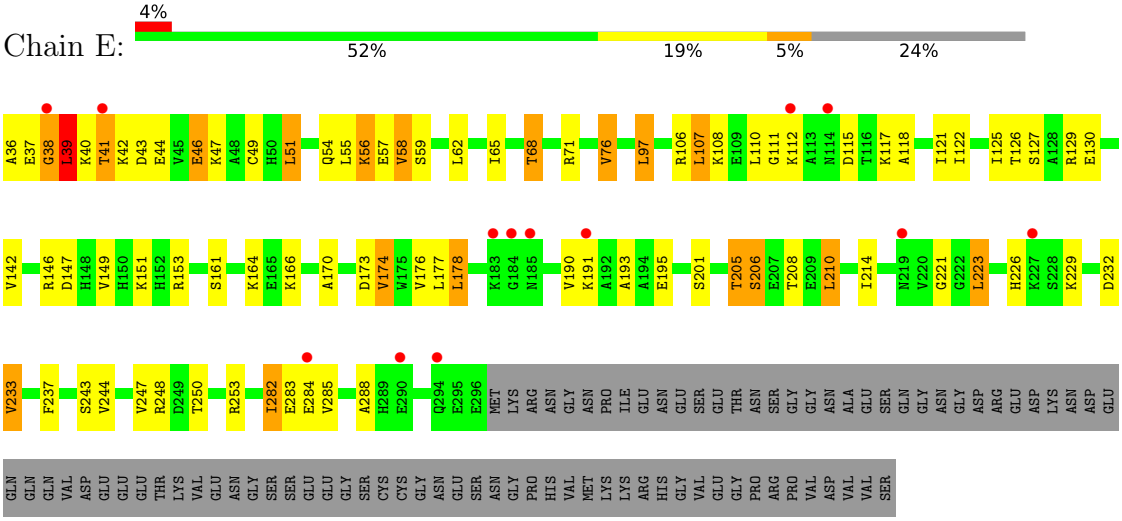
• Molecule 4: Iron-regulated surface determinant protein H

Chain 3:



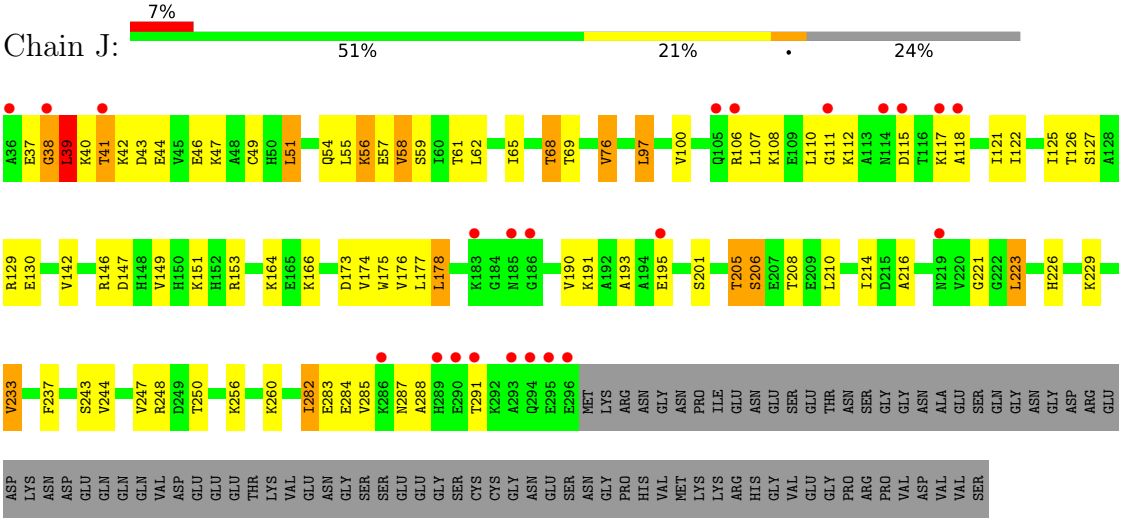
• Molecule 5: Haptoglobin-hemoglobin receptor

Chain E:



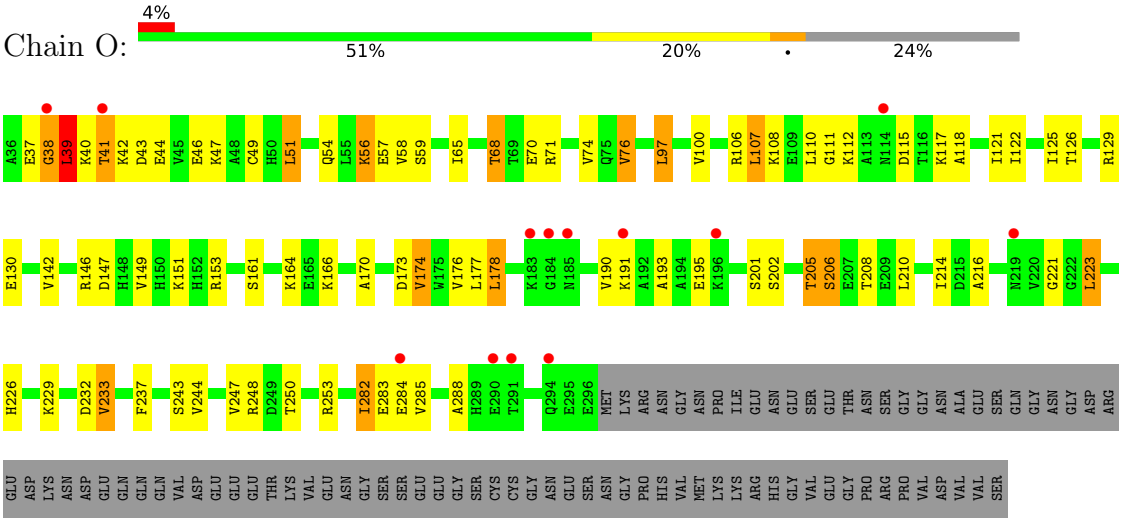
• Molecule 5: Haptoglobin-hemoglobin receptor

Chain J:



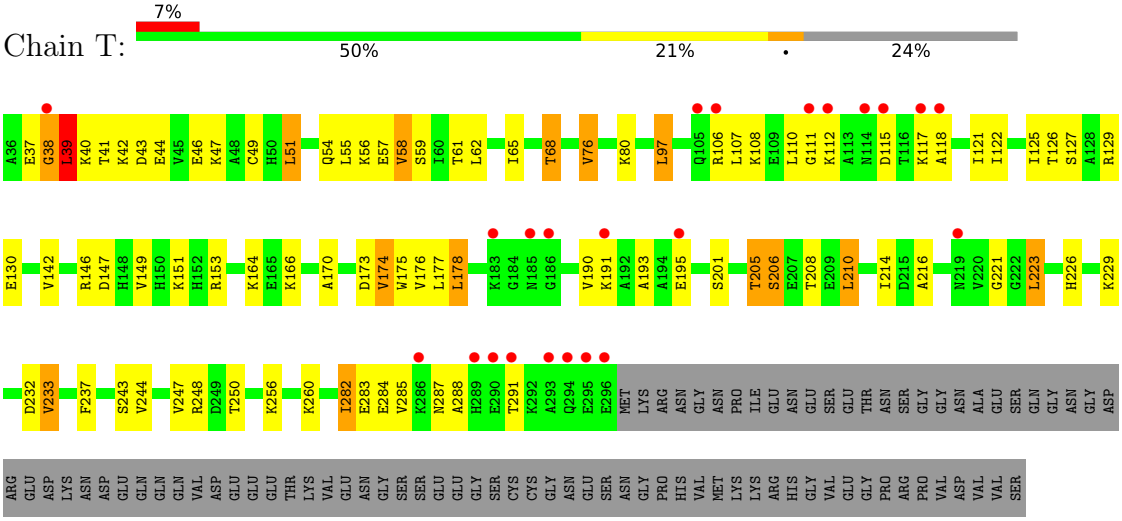
• Molecule 5: Haptoglobin-hemoglobin receptor

Chain O:



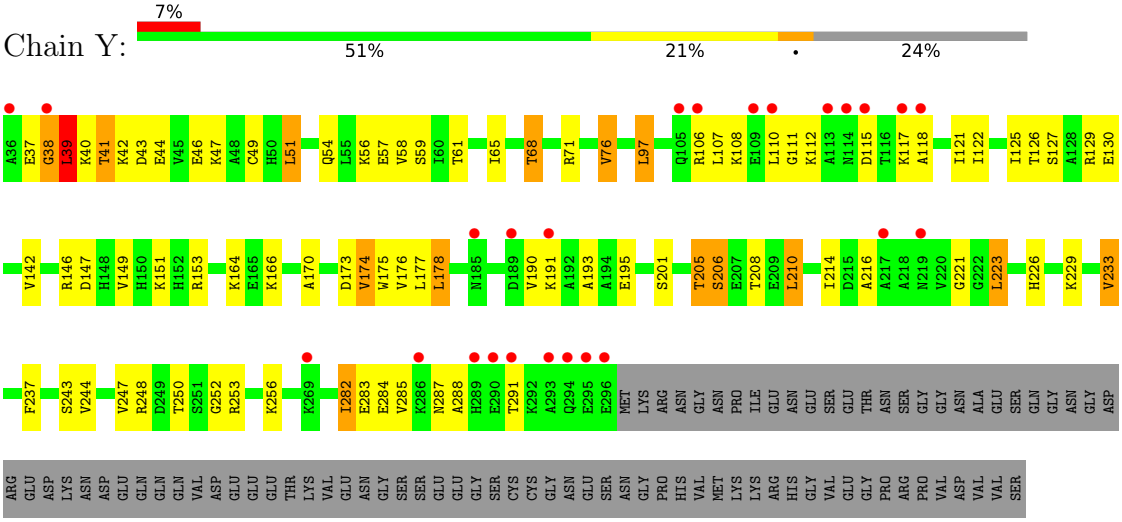
• Molecule 5: Haptoglobin-hemoglobin receptor

Chain T:



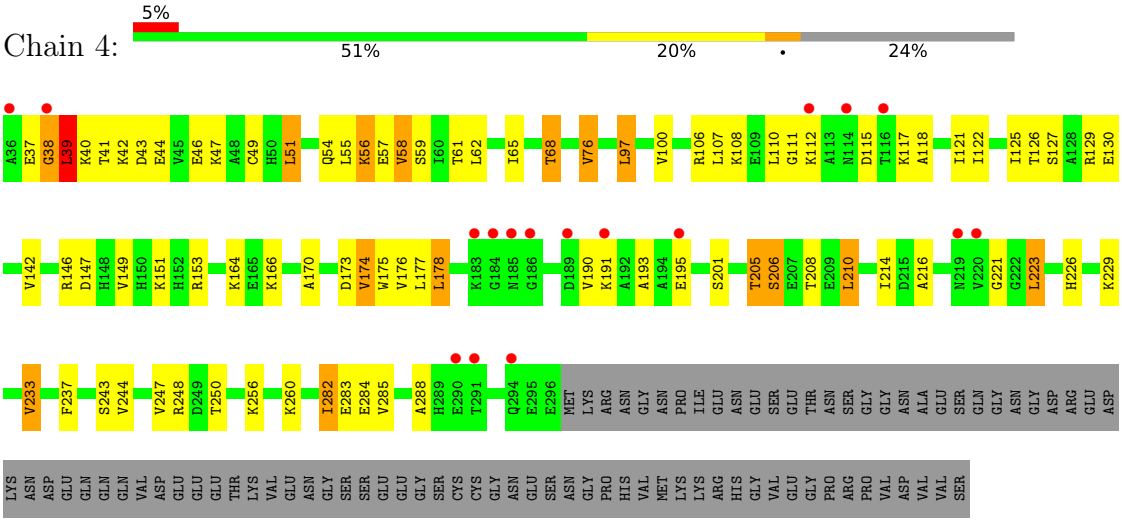
• Molecule 5: Haptoglobin-hemoglobin receptor

Chain Y:



• Molecule 5: Haptoglobin-hemoglobin receptor

Chain 4:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 50% 50%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j: 100%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	143.23Å 140.95Å 267.18Å 90.00° 98.54° 90.00°	Depositor
Resolution (Å)	29.00 – 3.10 28.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.1 (29.00-3.10) 96.7 (28.98-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.11Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.255 , 0.271 0.260 , 0.273	Depositor DCC
R_{free} test set	1758 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å^2)	65.7	Xtriage
Anisotropy	0.870	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	47792	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4672e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OXY, HEM, 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	0.54	0/1097	0.66	0/1491
1	F	0.52	0/1097	0.69	2/1491 (0.1%)
1	K	0.54	0/1097	0.68	0/1491
1	P	0.51	0/1097	0.64	0/1491
1	U	0.46	0/1097	0.61	0/1491
1	Z	0.47	0/1097	0.61	0/1491
2	1	0.49	0/1153	0.61	0/1566
2	B	0.59	0/1153	0.67	0/1566
2	G	0.57	0/1153	0.65	0/1566
2	L	0.59	0/1153	0.68	0/1566
2	Q	0.56	0/1153	0.65	0/1566
2	V	0.51	0/1153	0.61	0/1566
3	2	0.52	0/2497	0.71	0/3391
3	C	0.64	0/2497	0.77	0/3391
3	H	0.57	0/2497	0.74	0/3391
3	M	0.64	0/2497	0.77	0/3391
3	R	0.57	0/2497	0.74	0/3391
3	W	0.49	0/2497	0.71	0/3391
4	3	0.44	0/1212	0.62	0/1647
4	D	0.51	0/1212	0.66	0/1647
4	I	0.49	0/1212	0.65	0/1647
4	N	0.52	0/1212	0.66	0/1647
4	S	0.49	0/1212	0.65	0/1647
4	X	0.43	0/1212	0.63	0/1647
5	4	0.41	0/1981	0.62	1/2666 (0.0%)
5	E	0.45	0/1981	0.63	1/2666 (0.0%)
5	J	0.42	0/1981	0.62	1/2666 (0.0%)
5	O	0.48	0/1981	0.64	1/2666 (0.0%)
5	T	0.42	0/1981	0.62	1/2666 (0.0%)
5	Y	0.39	0/1981	0.61	1/2666 (0.0%)
All	All	0.52	0/47640	0.67	8/64566 (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	2	0	3
3	C	0	4
3	H	0	3
3	M	0	4
3	R	0	3
3	W	0	3
4	3	0	1
4	D	0	1
4	I	0	1
4	N	0	1
4	S	0	1
4	X	0	1
5	4	0	1
5	E	0	1
5	J	0	1
5	O	0	1
5	T	0	1
5	Y	0	1
All	All	0	32

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1	VAL	CG1-CB-CG2	6.10	120.66	110.90
1	F	1	VAL	CB-CA-C	-5.41	101.12	111.40
5	E	223	LEU	CA-CB-CG	5.25	127.38	115.30
5	T	223	LEU	CA-CB-CG	5.12	127.07	115.30
5	4	223	LEU	CA-CB-CG	5.09	127.01	115.30
5	Y	223	LEU	CA-CB-CG	5.08	126.98	115.30
5	O	223	LEU	CA-CB-CG	5.07	126.97	115.30
5	J	223	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	120	GLU	Peptide
3	2	311	GLY	Peptide
3	2	312	SER	Peptide
4	3	177	PRO	Peptide
5	4	38	GLY	Peptide
3	C	120	GLU	Peptide
3	C	311	GLY	Peptide
3	C	312	SER	Peptide
3	C	378	ALA	Peptide
4	D	177	PRO	Peptide
5	E	38	GLY	Peptide
3	H	120	GLU	Peptide
3	H	311	GLY	Peptide
3	H	312	SER	Peptide
4	I	177	PRO	Peptide
5	J	38	GLY	Peptide
3	M	120	GLU	Peptide
3	M	311	GLY	Peptide
3	M	312	SER	Peptide
3	M	378	ALA	Peptide
4	N	177	PRO	Peptide
5	O	38	GLY	Peptide
3	R	120	GLU	Peptide
3	R	311	GLY	Peptide
3	R	312	SER	Peptide
4	S	177	PRO	Peptide
5	T	38	GLY	Peptide
3	W	120	GLU	Peptide
3	W	311	GLY	Peptide
3	W	312	SER	Peptide
4	X	177	PRO	Peptide
5	Y	38	GLY	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	1069	0	1073	30	0
1	F	1069	0	1073	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1069	0	1073	30	0
1	P	1069	0	1073	24	0
1	U	1069	0	1073	33	0
1	Z	1069	0	1073	31	0
2	1	1123	0	1118	32	0
2	B	1123	0	1118	37	0
2	G	1123	0	1118	30	0
2	L	1123	0	1118	39	0
2	Q	1123	0	1118	34	0
2	V	1123	0	1118	33	0
3	2	2437	0	2388	93	0
3	C	2437	0	2387	103	0
3	H	2437	0	2388	99	0
3	M	2437	0	2387	102	0
3	R	2437	0	2387	102	0
3	W	2437	0	2388	94	0
4	3	1183	0	1132	16	0
4	D	1183	0	1132	19	0
4	I	1183	0	1132	17	0
4	N	1183	0	1132	18	0
4	S	1183	0	1132	17	0
4	X	1183	0	1132	17	0
5	4	1963	0	1978	57	0
5	E	1963	0	1978	65	0
5	J	1963	0	1978	60	0
5	O	1963	0	1978	58	0
5	T	1963	0	1978	58	0
5	Y	1963	0	1978	62	0
6	a	28	0	25	0	0
6	b	28	0	25	0	0
6	c	28	0	25	0	0
6	d	28	0	25	0	0
6	e	28	0	25	0	0
6	f	28	0	25	0	0
6	g	28	0	25	0	0
6	h	28	0	25	0	0
6	i	28	0	25	0	0
6	j	28	0	25	0	0
7	1	43	0	30	6	0
7	A	43	0	30	1	0
7	B	43	0	30	6	0
7	F	43	0	30	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	43	0	30	3	0
7	K	43	0	30	1	0
7	L	43	0	30	6	0
7	P	43	0	30	2	0
7	Q	43	0	30	4	0
7	U	43	0	30	4	0
7	V	43	0	30	3	0
7	Z	43	0	30	2	0
8	1	2	0	0	0	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	F	2	0	0	0	0
8	G	2	0	0	0	0
8	K	2	0	0	0	0
8	L	2	0	0	0	0
8	P	2	0	0	0	0
8	Q	2	0	0	0	0
8	U	2	0	0	1	0
8	V	2	0	0	1	0
8	Z	2	0	0	1	0
9	2	14	0	13	0	0
9	4	28	0	26	2	0
9	C	28	0	26	0	0
9	E	28	0	26	1	0
9	H	28	0	26	0	0
9	J	28	0	26	2	0
9	M	28	0	26	1	0
9	O	28	0	26	1	0
9	R	28	0	26	0	0
9	T	28	0	26	1	0
9	W	28	0	26	1	0
9	Y	28	0	26	1	0
All	All	47792	0	47040	1392	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 15.

All (1392) 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)
5:E:43:ASP:OD2	5:E:47:LYS:HE2	1.30	1.29

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:43:ASP:OD2	5:E:47:LYS:CE	2.15	0.94
3:2:183:THR:HB	3:2:199:ASN:HD22	1.36	0.89
3:M:183:THR:HB	3:M:199:ASN:HD22	1.35	0.89
5:O:57:GLU:HG3	5:O:201:SER:HB3	1.55	0.88
5:Y:57:GLU:HG3	5:Y:201:SER:HB3	1.57	0.87
3:C:188:ILE:HD11	3:C:263:LEU:HD21	1.57	0.86
3:C:183:THR:HB	3:C:199:ASN:HD22	1.39	0.86
3:M:188:ILE:HD11	3:M:263:LEU:HD21	1.57	0.85
5:T:57:GLU:HG3	5:T:201:SER:HB3	1.58	0.85
3:H:183:THR:HB	3:H:199:ASN:HD22	1.39	0.85
5:4:57:GLU:HG3	5:4:201:SER:HB3	1.57	0.85
3:R:183:THR:HB	3:R:199:ASN:HD22	1.41	0.84
1:Z:83:LEU:HD22	1:Z:87:HIS:HE1	1.43	0.84
5:J:57:GLU:HG3	5:J:201:SER:HB3	1.59	0.83
3:R:188:ILE:HD11	3:R:263:LEU:HD21	1.59	0.83
3:W:183:THR:HB	3:W:199:ASN:HD22	1.40	0.83
2:L:106:LEU:HD23	7:L:201:HEM:HBB2	1.60	0.83
3:W:188:ILE:HD11	3:W:263:LEU:HD21	1.60	0.83
1:F:83:LEU:HD22	1:F:87:HIS:HE1	1.44	0.83
1:U:83:LEU:HD22	1:U:87:HIS:HE1	1.44	0.82
5:E:57:GLU:HG3	5:E:201:SER:HB3	1.60	0.82
3:W:128:ASN:HB2	3:W:132:GLN:H	1.43	0.82
3:M:373:PHE:HB3	3:M:384:VAL:HG12	1.61	0.82
3:2:188:ILE:HD11	3:2:263:LEU:HD21	1.61	0.82
1:K:83:LEU:HD22	1:K:87:HIS:HE1	1.45	0.82
1:A:83:LEU:HD22	1:A:87:HIS:HE1	1.45	0.81
1:P:83:LEU:HD22	1:P:87:HIS:HE1	1.45	0.81
3:C:373:PHE:HB3	3:C:384:VAL:HG12	1.63	0.81
3:H:188:ILE:HD11	3:H:263:LEU:HD21	1.62	0.80
3:M:128:ASN:HB2	3:M:132:GLN:H	1.45	0.80
7:Q:201:HEM:HHC	7:Q:201:HEM:HBB2	1.62	0.80
3:H:128:ASN:HB2	3:H:132:GLN:H	1.44	0.80
3:C:128:ASN:HB2	3:C:132:GLN:H	1.46	0.80
3:2:373:PHE:HB3	3:2:384:VAL:HG12	1.63	0.80
3:W:373:PHE:HB3	3:W:384:VAL:HG12	1.64	0.80
3:2:128:ASN:HB2	3:2:132:GLN:H	1.45	0.79
5:E:43:ASP:O	5:E:46:GLU:HG3	1.82	0.79
3:R:128:ASN:HB2	3:R:132:GLN:H	1.45	0.78
3:R:373:PHE:HB3	3:R:384:VAL:HG12	1.64	0.78
2:G:24:GLY:H	2:G:68:LEU:HD22	1.50	0.77
5:O:40:LYS:HB3	5:O:44:GLU:HB3	1.64	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:9:ASN:HD22	1:Z:121:VAL:HG22	1.49	0.77
3:M:268:TYR:HB3	3:M:273:ARG:HG3	1.67	0.77
4:S:132:LYS:HB3	4:S:149:ASP:HB3	1.64	0.77
1:K:9:ASN:HD22	1:K:121:VAL:HG22	1.48	0.77
5:E:40:LYS:HB3	5:E:44:GLU:HB3	1.65	0.77
2:1:24:GLY:H	2:1:68:LEU:HD22	1.50	0.77
3:H:157:ASN:ND2	5:J:68:THR:O	2.18	0.77
5:J:40:LYS:HB3	5:J:44:GLU:HB3	1.64	0.77
3:W:268:TYR:HB3	3:W:273:ARG:HG3	1.67	0.77
1:F:9:ASN:HD22	1:F:121:VAL:HG22	1.50	0.76
4:N:132:LYS:HB3	4:N:149:ASP:HB3	1.67	0.76
5:4:40:LYS:HB3	5:4:44:GLU:HB3	1.64	0.76
5:Y:40:LYS:HB3	5:Y:44:GLU:HB3	1.65	0.76
3:H:373:PHE:HB3	3:H:384:VAL:HG12	1.67	0.76
2:B:24:GLY:H	2:B:68:LEU:HD22	1.50	0.76
2:L:24:GLY:H	2:L:68:LEU:HD22	1.50	0.76
2:V:24:GLY:HA3	2:V:68:LEU:HB2	1.66	0.76
2:G:24:GLY:HA3	2:G:68:LEU:HB2	1.66	0.76
3:H:268:TYR:HB3	3:H:273:ARG:HG3	1.66	0.76
5:T:40:LYS:HB3	5:T:44:GLU:HB3	1.65	0.76
2:V:24:GLY:H	2:V:68:LEU:HD22	1.51	0.75
4:D:132:LYS:HB3	4:D:149:ASP:HB3	1.68	0.75
1:U:9:ASN:HD22	1:U:121:VAL:HG22	1.52	0.75
4:I:132:LYS:HB3	4:I:149:ASP:HB3	1.68	0.75
1:K:101:LEU:HD23	7:K:201:HEM:HBB2	1.69	0.75
2:Q:24:GLY:HA3	2:Q:68:LEU:HB2	1.67	0.75
7:1:201:HEM:HHC	7:1:201:HEM:HBB2	1.69	0.75
3:C:315:PRO:HA	3:C:318:LYS:HG3	1.69	0.75
4:3:132:LYS:HB3	4:3:149:ASP:HB3	1.68	0.75
2:Q:24:GLY:H	2:Q:68:LEU:HD22	1.53	0.74
4:S:162:TYR:HB2	4:S:197:LYS:HB3	1.70	0.74
1:A:9:ASN:HD22	1:A:121:VAL:HG22	1.52	0.74
2:1:24:GLY:HA3	2:1:68:LEU:HB2	1.67	0.74
3:C:268:TYR:HB3	3:C:273:ARG:HG3	1.70	0.74
7:G:201:HEM:HHC	7:G:201:HEM:HBB2	1.68	0.74
5:T:147:ASP:OD2	5:T:151:LYS:NZ	2.19	0.74
4:D:162:TYR:HB2	4:D:197:LYS:HB3	1.68	0.74
4:X:132:LYS:HB3	4:X:149:ASP:HB3	1.68	0.74
5:4:147:ASP:OD2	5:4:151:LYS:NZ	2.19	0.74
2:L:41:PHE:CE2	2:L:98:VAL:HG22	2.23	0.73
4:N:162:TYR:HB2	4:N:197:LYS:HB3	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:9:ASN:HD22	1:P:121:VAL:HG22	1.53	0.73
3:M:315:PRO:HA	3:M:318:LYS:HG3	1.70	0.73
2:B:41:PHE:CE2	2:B:98:VAL:HG22	2.24	0.73
7:B:201:HEM:HBA2	7:B:201:HEM:HHA	1.71	0.73
2:L:24:GLY:HA3	2:L:68:LEU:HB2	1.68	0.72
5:O:59:SER:HB2	5:O:164:LYS:HG3	1.70	0.72
3:2:268:TYR:HB3	3:2:273:ARG:HG3	1.70	0.72
5:E:59:SER:HB2	5:E:164:LYS:HG3	1.70	0.72
4:I:162:TYR:HB2	4:I:197:LYS:HB3	1.72	0.72
4:3:162:TYR:HB2	4:3:197:LYS:HB3	1.72	0.72
3:C:261:ILE:HD13	3:C:367:ALA:HB2	1.72	0.72
3:R:268:TYR:HB3	3:R:273:ARG:HG3	1.70	0.72
3:C:178:HIS:HB2	3:C:216:THR:HG23	1.72	0.71
5:Y:147:ASP:OD2	5:Y:151:LYS:NZ	2.19	0.71
2:B:24:GLY:HA3	2:B:68:LEU:HB2	1.69	0.71
4:X:162:TYR:HB2	4:X:197:LYS:HB3	1.72	0.71
5:4:59:SER:HB2	5:4:164:LYS:HG3	1.72	0.71
3:2:178:HIS:HB2	3:2:216:THR:HG23	1.71	0.71
3:M:178:HIS:HB2	3:M:216:THR:HG23	1.72	0.70
3:H:315:PRO:HA	3:H:318:LYS:HG3	1.71	0.70
5:T:256:LYS:HE3	5:T:260:LYS:HE3	1.74	0.70
3:R:178:HIS:HB2	3:R:216:THR:HG23	1.72	0.70
3:R:315:PRO:HA	3:R:318:LYS:HG3	1.72	0.70
5:E:54:GLN:HE21	5:E:205:THR:HG23	1.57	0.69
3:W:315:PRO:HA	3:W:318:LYS:HG3	1.74	0.69
3:H:178:HIS:HB2	3:H:216:THR:HG23	1.73	0.69
5:T:247:VAL:HA	5:T:250:THR:HG22	1.75	0.69
2:B:41:PHE:HE2	2:B:98:VAL:HG22	1.57	0.69
2:L:41:PHE:HE2	2:L:98:VAL:HG22	1.56	0.69
3:M:261:ILE:HD13	3:M:367:ALA:HB2	1.74	0.69
3:M:196:THR:OG1	3:M:199:ASN:OD1	2.08	0.69
3:R:193:LEU:HD13	3:R:219:LEU:HD21	1.73	0.69
7:B:201:HEM:HHC	7:B:201:HEM:HBB2	1.75	0.69
3:2:315:PRO:HA	3:2:318:LYS:HG3	1.73	0.69
5:O:54:GLN:HE21	5:O:205:THR:HG23	1.58	0.68
4:S:86:ALA:N	4:S:88:GLU:OE2	2.26	0.68
3:W:178:HIS:HB2	3:W:216:THR:HG23	1.74	0.68
3:M:193:LEU:HD13	3:M:219:LEU:HD21	1.76	0.68
3:C:193:LEU:HD13	3:C:219:LEU:HD21	1.76	0.68
5:4:247:VAL:HA	5:4:250:THR:HG22	1.76	0.68
1:K:42:TYR:HE1	1:K:93:VAL:HA	1.59	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:163:GLU:HB3	4:D:168:LEU:HD21	1.75	0.68
5:E:247:VAL:HA	5:E:250:THR:HG22	1.74	0.68
2:Q:41:PHE:CE2	2:Q:98:VAL:HG22	2.29	0.68
1:Z:31:ARG:HD3	2:1:127:GLN:OE1	1.93	0.68
2:G:41:PHE:CE2	2:G:98:VAL:HG22	2.29	0.68
5:T:59:SER:HB2	5:T:164:LYS:HG3	1.75	0.68
5:O:247:VAL:HA	5:O:250:THR:HG22	1.75	0.67
5:J:147:ASP:OD2	5:J:151:LYS:NZ	2.18	0.67
1:A:42:TYR:HE1	1:A:93:VAL:HA	1.60	0.67
5:J:247:VAL:HA	5:J:250:THR:HG22	1.77	0.67
5:Y:54:GLN:HE21	5:Y:205:THR:HG23	1.59	0.67
5:E:115:ASP:HB3	5:E:118:ALA:HB3	1.75	0.67
5:J:59:SER:HB2	5:J:164:LYS:HG3	1.76	0.67
5:Y:247:VAL:HA	5:Y:250:THR:HG22	1.76	0.67
5:4:115:ASP:HB3	5:4:118:ALA:HB3	1.75	0.67
9:4:1002:NAG:O7	9:4:1002:NAG:O3	2.13	0.67
3:W:193:LEU:HD13	3:W:219:LEU:HD21	1.77	0.67
5:O:115:ASP:HB3	5:O:118:ALA:HB3	1.75	0.67
3:W:261:ILE:HD13	3:W:367:ALA:HB2	1.77	0.67
5:Y:68:THR:HG21	5:Y:248:ARG:HH21	1.60	0.67
3:C:196:THR:OG1	3:C:199:ASN:OD1	2.10	0.67
3:2:267:ASP:HB2	3:2:389:THR:HG21	1.77	0.67
3:C:267:ASP:HB2	3:C:389:THR:HG21	1.76	0.66
5:T:115:ASP:HB3	5:T:118:ALA:HB3	1.76	0.66
5:4:68:THR:HG21	5:4:248:ARG:HH21	1.61	0.66
5:J:54:GLN:HE21	5:J:205:THR:HG23	1.60	0.66
5:Y:59:SER:HB2	5:Y:164:LYS:HG3	1.76	0.66
4:D:86:ALA:N	4:D:88:GLU:OE2	2.28	0.66
3:H:261:ILE:HD13	3:H:367:ALA:HB2	1.78	0.66
5:Y:115:ASP:HB3	5:Y:118:ALA:HB3	1.77	0.66
5:E:43:ASP:CG	5:E:47:LYS:HE2	2.14	0.66
3:M:109:TYR:OH	3:R:96:PRO:O	2.09	0.66
3:M:267:ASP:HB2	3:M:389:THR:HG21	1.76	0.66
3:R:261:ILE:HD13	3:R:367:ALA:HB2	1.78	0.66
5:Y:166:LYS:HB3	5:Y:233:VAL:HG12	1.78	0.66
3:2:193:LEU:HD13	3:2:219:LEU:HD21	1.77	0.66
5:4:117:LYS:NZ	5:4:284:GLU:OE1	2.28	0.65
4:I:86:ALA:N	4:I:88:GLU:OE2	2.30	0.65
4:X:173:VAL:HG11	4:X:186:ARG:HD2	1.78	0.65
4:3:163:GLU:HB3	4:3:168:LEU:HD21	1.78	0.65
3:H:193:LEU:HD13	3:H:219:LEU:HD21	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:267:ASP:HB2	3:H:389:THR:HG21	1.79	0.65
5:J:39:LEU:H	5:J:223:LEU:HD11	1.61	0.65
5:T:39:LEU:H	5:T:223:LEU:HD11	1.61	0.65
3:C:345:ASP:CG	3:C:346:THR:H	2.00	0.65
4:X:163:GLU:HB3	4:X:168:LEU:HD21	1.78	0.65
5:J:115:ASP:HB3	5:J:118:ALA:HB3	1.77	0.65
2:V:41:PHE:CE2	2:V:98:VAL:HG22	2.32	0.65
3:R:345:ASP:CG	3:R:346:THR:H	1.99	0.65
3:M:351:ALA:HA	3:M:371:LEU:HB3	1.77	0.65
5:O:147:ASP:OD2	5:O:151:LYS:NZ	2.21	0.65
5:E:39:LEU:H	5:E:223:LEU:HD11	1.62	0.65
3:R:351:ALA:HA	3:R:371:LEU:HB3	1.77	0.64
3:W:128:ASN:HB3	3:W:130:GLU:H	1.61	0.64
3:M:223:LYS:HD3	3:M:257:ARG:HH11	1.60	0.64
4:S:163:GLU:HB3	4:S:168:LEU:HD21	1.79	0.64
3:W:267:ASP:HB2	3:W:389:THR:HG21	1.77	0.64
1:P:31:ARG:HD3	2:Q:127:GLN:OE1	1.98	0.64
3:R:267:ASP:HB2	3:R:389:THR:HG21	1.80	0.64
5:T:166:LYS:HB3	5:T:233:VAL:HG12	1.79	0.64
3:H:196:THR:OG1	3:H:199:ASN:OD1	2.10	0.64
3:M:264:PRO:HB2	3:M:266:LYS:O	1.98	0.64
4:N:163:GLU:HB3	4:N:168:LEU:HD21	1.79	0.64
5:4:54:GLN:HE21	5:4:205:THR:HG23	1.63	0.64
5:E:166:LYS:HB3	5:E:233:VAL:HG12	1.80	0.64
3:M:345:ASP:CG	3:M:346:THR:H	2.01	0.64
4:N:86:ALA:N	4:N:88:GLU:OE2	2.30	0.64
7:P:201:HEM:HBB2	7:P:201:HEM:HMB1	1.80	0.64
1:U:42:TYR:HE1	1:U:93:VAL:HA	1.63	0.64
4:I:163:GLU:HB3	4:I:168:LEU:HD21	1.80	0.64
1:U:31:ARG:HD3	2:V:127:GLN:OE1	1.97	0.64
4:X:86:ALA:N	4:X:88:GLU:OE2	2.30	0.64
5:4:39:LEU:H	5:4:223:LEU:HD11	1.62	0.64
1:K:31:ARG:HD3	2:L:127:GLN:OE1	1.97	0.64
2:1:41:PHE:CE2	2:1:98:VAL:HG22	2.33	0.64
3:C:223:LYS:HD3	3:C:257:ARG:HH11	1.61	0.64
5:J:68:THR:HG21	5:J:248:ARG:HH21	1.62	0.64
3:M:174:LYS:HB2	3:M:280:TRP:CD1	2.33	0.64
3:R:128:ASN:HB3	3:R:130:GLU:H	1.63	0.63
5:E:147:ASP:OD2	5:E:151:LYS:NZ	2.21	0.63
3:M:128:ASN:HB3	3:M:130:GLU:H	1.62	0.63
5:Y:39:LEU:H	5:Y:223:LEU:HD11	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:351:ALA:HA	3:W:371:LEU:HB3	1.79	0.63
1:Z:42:TYR:HE1	1:Z:93:VAL:HA	1.63	0.63
3:H:128:ASN:HB3	3:H:130:GLU:H	1.64	0.63
4:S:173:VAL:HG11	4:S:186:ARG:HD2	1.80	0.63
4:3:86:ALA:N	4:3:88:GLU:OE2	2.32	0.63
1:F:42:TYR:HE1	1:F:93:VAL:HA	1.63	0.63
5:O:117:LYS:NZ	5:O:284:GLU:OE1	2.29	0.63
4:D:173:VAL:HG11	4:D:186:ARG:HD2	1.81	0.63
3:H:223:LYS:HD3	3:H:257:ARG:HH11	1.61	0.63
2:L:25:GLY:HA2	2:L:64:GLY:HA3	1.81	0.63
3:M:119:THR:HG23	3:M:121:GLY:HA3	1.81	0.63
5:T:54:GLN:HE21	5:T:205:THR:HG23	1.64	0.63
3:2:261:ILE:HD13	3:2:367:ALA:HB2	1.80	0.63
2:G:95:LYS:HE3	5:J:201:SER:O	1.98	0.62
5:J:117:LYS:NZ	5:J:284:GLU:OE1	2.30	0.62
3:2:128:ASN:HB3	3:2:130:GLU:H	1.64	0.62
3:M:142:LEU:HD11	3:R:96:PRO:HG2	1.80	0.62
1:K:42:TYR:CE1	1:K:93:VAL:HA	2.33	0.62
5:O:166:LYS:HB3	5:O:233:VAL:HG12	1.82	0.62
1:A:31:ARG:HD3	2:B:127:GLN:OE1	1.99	0.62
1:A:98:PHE:HB3	1:A:133:SER:OG	1.99	0.62
5:E:117:LYS:NZ	5:E:284:GLU:OE1	2.30	0.62
5:T:117:LYS:NZ	5:T:284:GLU:OE1	2.31	0.62
7:1:201:HEM:HHD	7:1:201:HEM:HBC2	1.82	0.62
5:E:46:GLU:O	5:E:49:CYS:N	2.32	0.62
1:A:42:TYR:CE1	1:A:93:VAL:HA	2.34	0.62
5:T:68:THR:HG21	5:T:248:ARG:HH21	1.64	0.62
3:2:351:ALA:HA	3:2:371:LEU:HB3	1.80	0.62
7:L:201:HEM:HHD	7:L:201:HEM:HBC2	1.81	0.62
4:N:173:VAL:HG11	4:N:186:ARG:HD2	1.82	0.62
5:O:39:LEU:H	5:O:223:LEU:HD11	1.64	0.62
3:2:223:LYS:HD3	3:2:257:ARG:HH11	1.63	0.62
5:E:126:THR:O	5:E:130:GLU:HG2	2.00	0.61
3:H:351:ALA:HA	3:H:371:LEU:HB3	1.81	0.61
5:O:68:THR:HG21	5:O:248:ARG:HH21	1.65	0.61
2:V:95:LYS:HE3	5:Y:201:SER:O	1.99	0.61
3:W:223:LYS:HD3	3:W:257:ARG:HH11	1.63	0.61
5:J:39:LEU:N	5:J:223:LEU:HD21	2.15	0.61
2:1:25:GLY:HA2	2:1:64:GLY:HA3	1.82	0.61
3:W:196:THR:OG1	3:W:199:ASN:OD1	2.14	0.61
3:2:196:THR:OG1	3:2:199:ASN:OD1	2.14	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:ARG:HD3	2:G:127:GLN:OE1	2.01	0.61
3:W:142:LEU:HD11	3:2:96:PRO:HG2	1.82	0.61
2:B:25:GLY:HA2	2:B:64:GLY:HA3	1.83	0.61
2:L:19:ASN:ND2	2:L:22:GLU:HB2	2.16	0.61
3:C:264:PRO:HB2	3:C:266:LYS:O	2.01	0.61
1:F:84:SER:HB3	1:F:139:LYS:HD2	1.82	0.61
3:R:223:LYS:HD3	3:R:257:ARG:HH11	1.64	0.61
3:H:345:ASP:CG	3:H:346:THR:H	2.03	0.61
5:Y:117:LYS:NZ	5:Y:284:GLU:OE1	2.30	0.61
5:E:68:THR:HG21	5:E:248:ARG:HH21	1.66	0.61
3:C:130:GLU:N	3:C:130:GLU:OE1	2.34	0.60
1:K:17:VAL:HG13	1:K:24:TYR:CE1	2.35	0.60
4:3:173:VAL:HG11	4:3:186:ARG:HD2	1.82	0.60
3:C:119:THR:HG23	3:C:121:GLY:HA3	1.83	0.60
3:C:145:CYS:HB2	3:H:99:ALA:O	2.01	0.60
2:G:25:GLY:HA2	2:G:64:GLY:HA3	1.83	0.60
5:E:110:LEU:HD21	5:E:288:ALA:HB1	1.83	0.60
1:U:42:TYR:CE1	1:U:93:VAL:HA	2.36	0.60
1:F:98:PHE:HB3	1:F:133:SER:OG	2.02	0.60
3:M:336:CYS:SG	3:M:384:VAL:HG23	2.42	0.60
5:Y:110:LEU:HD21	5:Y:288:ALA:HB1	1.83	0.60
3:2:345:ASP:CG	3:2:346:THR:H	2.03	0.60
2:L:95:LYS:HE3	5:O:201:SER:O	2.02	0.60
1:F:42:TYR:CE1	1:F:93:VAL:HA	2.36	0.60
1:P:42:TYR:HE1	1:P:93:VAL:HA	1.66	0.60
5:T:39:LEU:N	5:T:223:LEU:HD21	2.16	0.60
5:4:39:LEU:N	5:4:223:LEU:HD21	2.16	0.60
2:Q:25:GLY:HA2	2:Q:64:GLY:HA3	1.83	0.60
3:M:145:CYS:HB2	3:R:99:ALA:O	2.01	0.60
2:Q:41:PHE:HE2	2:Q:98:VAL:HG22	1.66	0.60
3:W:345:ASP:CG	3:W:346:THR:H	2.05	0.60
3:C:373:PHE:CB	3:C:384:VAL:HG12	2.32	0.60
4:I:173:VAL:HG11	4:I:186:ARG:HD2	1.83	0.60
5:J:110:LEU:HD21	5:J:288:ALA:HB1	1.83	0.60
5:Y:39:LEU:N	5:Y:223:LEU:HD21	2.17	0.60
1:Z:42:TYR:CE1	1:Z:93:VAL:HA	2.36	0.60
3:C:128:ASN:HB3	3:C:130:GLU:H	1.66	0.59
1:Z:17:VAL:HG13	1:Z:24:TYR:CE1	2.36	0.59
3:2:174:LYS:HB2	3:2:280:TRP:CD1	2.37	0.59
3:C:142:LEU:HD11	3:H:96:PRO:HG2	1.83	0.59
2:L:106:LEU:HD23	7:L:201:HEM:CBB	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:41:PHE:HE2	2:V:98:VAL:HG22	1.66	0.59
5:4:110:LEU:HD21	5:4:288:ALA:HB1	1.83	0.59
5:O:39:LEU:N	5:O:223:LEU:HD21	2.17	0.59
3:R:219:LEU:HD12	3:R:220:TYR:H	1.68	0.59
5:T:110:LEU:HD21	5:T:288:ALA:HB1	1.83	0.59
2:V:25:GLY:HA2	2:V:64:GLY:HA3	1.84	0.59
5:O:110:LEU:HD21	5:O:288:ALA:HB1	1.83	0.59
3:M:151:LYS:H	3:M:259:MET:CE	2.16	0.59
2:Q:95:LYS:HE3	5:T:201:SER:O	2.01	0.59
2:1:95:LYS:HE3	5:4:201:SER:O	2.03	0.59
1:U:58:HIS:NE2	8:U:202:OXY:O1	2.36	0.59
5:E:39:LEU:N	5:E:223:LEU:HD21	2.18	0.59
3:H:350:ASP:O	3:H:371:LEU:HD12	2.03	0.59
3:W:174:LYS:HB2	3:W:280:TRP:CD1	2.38	0.59
3:C:186:THR:HG21	3:C:354:ALA:HB2	1.84	0.58
5:J:38:GLY:HA2	5:J:223:LEU:HG	1.85	0.58
3:R:174:LYS:HB2	3:R:280:TRP:CD1	2.37	0.58
3:H:335:PHE:HD2	3:H:387:LYS:HG2	1.67	0.58
5:J:221:GLY:C	5:J:223:LEU:H	2.05	0.58
1:K:84:SER:HB3	1:K:139:LYS:HD2	1.86	0.58
2:B:19:ASN:ND2	2:B:22:GLU:HB2	2.19	0.58
1:A:17:VAL:HG13	1:A:24:TYR:CE1	2.37	0.58
2:G:41:PHE:HE2	2:G:98:VAL:HG22	1.67	0.58
2:L:97:HIS:HB3	3:M:163:LEU:HD12	1.85	0.58
1:P:42:TYR:CE1	1:P:93:VAL:HA	2.38	0.58
5:E:36:ALA:N	3:R:238:TYR:HH	2.02	0.58
1:K:98:PHE:HB3	1:K:133:SER:OG	2.03	0.58
2:B:97:HIS:HB3	3:C:163:LEU:HD12	1.85	0.58
3:R:335:PHE:HD2	3:R:387:LYS:HG2	1.67	0.58
3:W:186:THR:HG21	3:W:354:ALA:HB2	1.85	0.58
5:O:282:ILE:HG12	5:O:285:VAL:HG11	1.86	0.58
5:T:38:GLY:HA2	5:T:223:LEU:HG	1.85	0.58
5:T:221:GLY:C	5:T:223:LEU:H	2.06	0.58
5:E:282:ILE:HG12	5:E:285:VAL:HG11	1.86	0.57
5:Y:221:GLY:C	5:Y:223:LEU:H	2.06	0.57
3:2:219:LEU:HD12	3:2:220:TYR:H	1.69	0.57
5:E:43:ASP:O	5:E:46:GLU:CG	2.53	0.57
5:Y:146:ARG:O	5:Y:149:VAL:HG12	2.04	0.57
3:C:371:LEU:HD13	3:C:385:TYR:CE2	2.39	0.57
5:E:76:VAL:HG21	5:E:146:ARG:HA	1.86	0.57
3:M:186:THR:HG21	3:M:354:ALA:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:56:LYS:NZ	5:O:59:SER:OG	2.37	0.57
7:Q:201:HEM:HBC2	7:Q:201:HEM:HHD	1.86	0.57
1:U:17:VAL:HG13	1:U:24:TYR:CE1	2.38	0.57
3:W:179:HIS:HB3	9:W:1002:NAG:H83	1.86	0.57
5:Y:107:LEU:HD22	5:Y:111:GLY:HA3	1.86	0.57
1:F:17:VAL:HG13	1:F:24:TYR:CE1	2.38	0.57
5:J:107:LEU:HD22	5:J:111:GLY:HA3	1.86	0.57
3:C:174:LYS:HB2	3:C:280:TRP:CD1	2.39	0.57
3:H:119:THR:HG23	3:H:121:GLY:HA3	1.85	0.57
3:H:255:ASN:OD1	3:H:257:ARG:HG2	2.05	0.57
3:M:219:LEU:HD12	3:M:220:TYR:H	1.69	0.57
1:P:84:SER:HB3	1:P:139:LYS:HD2	1.85	0.57
5:T:107:LEU:HD22	5:T:111:GLY:HA3	1.87	0.57
2:G:19:ASN:ND2	2:G:22:GLU:HB2	2.20	0.57
3:H:174:LYS:HB2	3:H:280:TRP:CD1	2.39	0.57
5:O:107:LEU:HD22	5:O:111:GLY:HA3	1.87	0.57
2:Q:19:ASN:ND2	2:Q:22:GLU:HB2	2.20	0.57
1:Z:11:LYS:NZ	4:3:151:ASN:OD1	2.38	0.57
1:Z:58:HIS:NE2	8:Z:202:OXY:O1	2.38	0.57
3:H:151:LYS:H	3:H:259:MET:CE	2.18	0.57
1:P:98:PHE:HB3	1:P:133:SER:OG	2.05	0.57
3:R:350:ASP:O	3:R:371:LEU:HD12	2.05	0.57
1:U:3:SER:N	1:U:6:ASP:OD2	2.36	0.57
5:Y:282:ILE:HG12	5:Y:285:VAL:HG11	1.86	0.57
5:4:51:LEU:HD21	5:4:214:ILE:HD13	1.86	0.57
9:T:1002:NAG:O7	9:T:1002:NAG:O3	2.16	0.57
3:W:219:LEU:HD12	3:W:220:TYR:H	1.68	0.57
5:E:107:LEU:HD22	5:E:111:GLY:HA3	1.87	0.57
5:O:76:VAL:HG21	5:O:146:ARG:HA	1.86	0.57
3:R:373:PHE:CB	3:R:384:VAL:HG12	2.33	0.57
5:T:206:SER:HB3	5:T:208:THR:H	1.70	0.57
5:4:38:GLY:HA2	5:4:223:LEU:HG	1.86	0.57
7:L:201:HEM:HBA2	7:L:201:HEM:HHA	1.87	0.56
3:R:221:VAL:HG23	3:R:225:GLN:HB3	1.86	0.56
2:1:41:PHE:HE2	2:1:98:VAL:HG22	1.70	0.56
5:4:221:GLY:C	5:4:223:LEU:H	2.07	0.56
3:C:219:LEU:HD12	3:C:220:TYR:H	1.70	0.56
3:C:335:PHE:HD2	3:C:387:LYS:HG2	1.69	0.56
5:E:206:SER:HB3	5:E:208:THR:H	1.69	0.56
7:1:201:HEM:HBA2	7:1:201:HEM:HHA	1.87	0.56
3:M:335:PHE:HD2	3:M:387:LYS:HG2	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:221:GLY:C	5:O:223:LEU:H	2.07	0.56
2:Q:122:PHE:CE2	2:Q:127:GLN:HB2	2.40	0.56
3:W:335:PHE:HD2	3:W:387:LYS:HG2	1.70	0.56
3:2:183:THR:HB	3:2:199:ASN:ND2	2.16	0.56
3:H:219:LEU:HD12	3:H:220:TYR:H	1.70	0.56
3:M:350:ASP:O	3:M:371:LEU:HD12	2.06	0.56
5:T:146:ARG:O	5:T:149:VAL:HG12	2.05	0.56
3:2:373:PHE:CB	3:2:384:VAL:HG12	2.34	0.56
5:E:221:GLY:C	5:E:223:LEU:H	2.08	0.56
7:G:201:HEM:HHD	7:G:201:HEM:HBC2	1.88	0.56
1:P:44:PRO:HB2	1:P:45:HIS:ND1	2.20	0.56
3:R:230:GLU:HB2	3:R:249:LYS:HA	1.87	0.56
2:V:97:HIS:HB3	3:W:163:LEU:HD12	1.87	0.56
5:Y:76:VAL:HG21	5:Y:146:ARG:HA	1.87	0.56
1:F:44:PRO:HB2	1:F:45:HIS:ND1	2.20	0.56
1:K:44:PRO:HB2	1:K:45:HIS:ND1	2.20	0.56
1:P:17:VAL:HG13	1:P:24:TYR:CE1	2.40	0.56
3:R:255:ASN:OD1	3:R:257:ARG:HG2	2.06	0.56
5:J:76:VAL:HG21	5:J:146:ARG:HA	1.87	0.56
3:M:221:VAL:HG23	3:M:225:GLN:HB3	1.86	0.56
5:O:146:ARG:O	5:O:149:VAL:HG12	2.04	0.56
3:R:186:THR:HG21	3:R:354:ALA:HB2	1.88	0.56
5:Y:38:GLY:HA2	5:Y:223:LEU:HG	1.87	0.56
2:1:19:ASN:ND2	2:1:22:GLU:HB2	2.21	0.56
5:J:282:ILE:HG12	5:J:285:VAL:HG11	1.86	0.56
5:O:38:GLY:HA2	5:O:223:LEU:HG	1.85	0.56
5:O:65:ILE:HG22	5:O:244:VAL:HG21	1.87	0.56
5:4:146:ARG:O	5:4:149:VAL:HG12	2.05	0.56
1:A:44:PRO:HB2	1:A:45:HIS:ND1	2.20	0.56
5:T:282:ILE:HG12	5:T:285:VAL:HG11	1.86	0.56
1:Z:98:PHE:HB3	1:Z:133:SER:OG	2.06	0.56
5:4:282:ILE:HG12	5:4:285:VAL:HG11	1.87	0.56
5:J:108:LYS:HA	5:J:112:LYS:HG2	1.88	0.56
3:M:130:GLU:N	3:M:130:GLU:OE1	2.39	0.56
5:4:107:LEU:HD22	5:4:111:GLY:HA3	1.88	0.56
3:M:186:THR:HG23	3:M:352:GLY:O	2.06	0.55
5:T:51:LEU:HD21	5:T:214:ILE:HD13	1.88	0.55
5:T:108:LYS:HA	5:T:112:LYS:HG2	1.88	0.55
2:V:63:HIS:NE2	8:V:202:OXY:O1	2.40	0.55
3:W:119:THR:HG23	3:W:121:GLY:HA3	1.88	0.55
3:W:264:PRO:HB2	3:W:266:LYS:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:151:LYS:H	3:2:259:MET:CE	2.19	0.55
1:A:92:ARG:NH1	1:A:141:ARG:O	2.38	0.55
3:R:128:ASN:HB3	3:R:130:GLU:N	2.21	0.55
5:T:76:VAL:HG21	5:T:146:ARG:HA	1.88	0.55
2:1:97:HIS:HB3	3:2:163:LEU:HD12	1.88	0.55
3:C:151:LYS:H	3:C:259:MET:CE	2.19	0.55
5:J:206:SER:HB3	5:J:208:THR:H	1.72	0.55
5:O:126:THR:O	5:O:130:GLU:HG2	2.07	0.55
5:Y:51:LEU:HD21	5:Y:214:ILE:HD13	1.88	0.55
3:2:119:THR:HG23	3:2:121:GLY:HA3	1.87	0.55
1:K:92:ARG:NH1	1:K:141:ARG:O	2.39	0.55
2:B:95:LYS:HE3	5:E:201:SER:O	2.07	0.55
5:T:173:ASP:O	5:T:176:VAL:HG12	2.06	0.55
5:Y:173:ASP:O	5:Y:176:VAL:HG12	2.06	0.55
5:4:206:SER:HB3	5:4:208:THR:H	1.72	0.55
3:H:128:ASN:HB3	3:H:130:GLU:N	2.22	0.55
5:J:146:ARG:O	5:J:149:VAL:HG12	2.06	0.55
3:R:120:GLU:N	3:R:121:GLY:HA3	2.21	0.55
1:F:3:SER:N	1:F:6:ASP:OD2	2.35	0.55
3:H:373:PHE:CB	3:H:384:VAL:HG12	2.36	0.55
1:U:92:ARG:NH1	1:U:141:ARG:O	2.39	0.55
2:B:106:LEU:HD23	7:B:201:HEM:CBB	2.37	0.55
3:H:230:GLU:HB2	3:H:249:LYS:HA	1.89	0.55
3:2:130:GLU:N	3:2:130:GLU:OE1	2.40	0.55
5:E:38:GLY:HA2	5:E:223:LEU:HG	1.87	0.54
3:H:186:THR:HG21	3:H:354:ALA:HB2	1.89	0.54
5:4:76:VAL:HG21	5:4:146:ARG:HA	1.89	0.54
1:A:6:ASP:O	1:A:10:VAL:HG23	2.07	0.54
2:B:106:LEU:HD23	7:B:201:HEM:HBB2	1.88	0.54
3:C:371:LEU:HD13	3:C:385:TYR:CZ	2.43	0.54
5:J:221:GLY:C	5:J:223:LEU:N	2.61	0.54
5:O:51:LEU:HD21	5:O:214:ILE:HD13	1.88	0.54
3:R:119:THR:HG23	3:R:121:GLY:HA3	1.88	0.54
5:Y:47:LYS:HD3	5:Y:216:ALA:O	2.08	0.54
4:D:158:LYS:O	4:D:200:SER:HA	2.07	0.54
3:H:130:GLU:N	3:H:130:GLU:OE1	2.40	0.54
3:M:254:VAL:HG13	3:M:259:MET:HB2	1.88	0.54
5:O:47:LYS:HD3	5:O:216:ALA:O	2.08	0.54
5:Y:126:THR:O	5:Y:130:GLU:HG2	2.08	0.54
3:C:230:GLU:HB2	3:C:249:LYS:HA	1.89	0.54
3:M:230:GLU:HB2	3:M:249:LYS:HA	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:186:THR:HG23	3:R:352:GLY:O	2.07	0.54
5:T:65:ILE:HG22	5:T:244:VAL:HG21	1.89	0.54
5:T:221:GLY:C	5:T:223:LEU:N	2.61	0.54
2:V:122:PHE:CE2	2:V:127:GLN:HB2	2.42	0.54
5:Y:108:LYS:HA	5:Y:112:LYS:HG2	1.88	0.54
1:Z:84:SER:HB3	1:Z:139:LYS:HD2	1.88	0.54
3:C:184:GLY:O	3:C:352:GLY:HA3	2.08	0.54
3:H:254:VAL:HG13	3:H:259:MET:HB2	1.89	0.54
1:F:129:LEU:O	1:F:133:SER:HB2	2.08	0.54
3:H:264:PRO:HB2	3:H:266:LYS:O	2.07	0.54
3:M:337:ALA:HB3	3:M:385:TYR:HE1	1.73	0.54
5:O:226:HIS:O	5:O:229:LYS:HG2	2.08	0.54
3:W:230:GLU:HB2	3:W:249:LYS:HA	1.90	0.54
3:2:230:GLU:HB2	3:2:249:LYS:HA	1.89	0.54
4:3:194:GLN:HG3	4:3:222:PRO:HA	1.90	0.54
5:E:146:ARG:O	5:E:149:VAL:HG12	2.07	0.54
5:J:191:LYS:NZ	5:J:195:GLU:OE2	2.40	0.54
3:M:373:PHE:CB	3:M:384:VAL:HG12	2.32	0.54
3:R:130:GLU:N	3:R:130:GLU:OE1	2.41	0.54
5:E:56:LYS:NZ	5:E:59:SER:OG	2.41	0.54
5:E:173:ASP:O	5:E:176:VAL:HG12	2.07	0.54
3:M:162:HIS:HB3	3:M:294:TYR:CE2	2.42	0.54
3:M:188:ILE:HG12	3:M:263:LEU:HD11	1.90	0.54
5:T:126:THR:O	5:T:130:GLU:HG2	2.08	0.54
1:A:84:SER:HB3	1:A:139:LYS:HD2	1.90	0.54
3:C:254:VAL:HG13	3:C:259:MET:HB2	1.88	0.54
5:J:51:LEU:HD21	5:J:214:ILE:HD13	1.90	0.54
5:J:226:HIS:O	5:J:229:LYS:HG2	2.07	0.54
3:M:128:ASN:HB3	3:M:130:GLU:N	2.22	0.54
3:M:142:LEU:HD11	3:R:96:PRO:CG	2.38	0.54
5:O:173:ASP:O	5:O:176:VAL:HG12	2.07	0.54
5:Y:221:GLY:C	5:Y:223:LEU:N	2.61	0.54
3:2:335:PHE:HD2	3:2:387:LYS:HG2	1.72	0.54
5:4:173:ASP:O	5:4:176:VAL:HG12	2.07	0.54
3:C:186:THR:HG23	3:C:352:GLY:O	2.08	0.54
3:H:221:VAL:HG23	3:H:225:GLN:HB3	1.89	0.54
3:W:151:LYS:H	3:W:259:MET:CE	2.20	0.54
3:2:186:THR:HG21	3:2:354:ALA:HB2	1.90	0.54
1:F:92:ARG:NH1	1:F:141:ARG:O	2.40	0.53
2:G:122:PHE:CE2	2:G:127:GLN:HB2	2.43	0.53
3:H:151:LYS:H	3:H:259:MET:HE1	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:271:VAL:HA	3:H:299:VAL:HG22	1.89	0.53
5:J:47:LYS:HD3	5:J:216:ALA:O	2.08	0.53
5:J:173:ASP:O	5:J:176:VAL:HG12	2.07	0.53
5:E:65:ILE:HG22	5:E:244:VAL:HG21	1.91	0.53
1:P:92:ARG:NH1	1:P:141:ARG:O	2.41	0.53
5:T:47:LYS:HD3	5:T:216:ALA:O	2.07	0.53
3:2:128:ASN:HB3	3:2:130:GLU:N	2.23	0.53
3:2:255:ASN:OD1	3:2:257:ARG:HG2	2.09	0.53
3:W:254:VAL:HG13	3:W:259:MET:HB2	1.89	0.53
3:2:221:VAL:HG23	3:2:225:GLN:HB3	1.90	0.53
3:2:264:PRO:HB2	3:2:266:LYS:O	2.08	0.53
5:4:65:ILE:HG22	5:4:244:VAL:HG21	1.90	0.53
5:E:51:LEU:HD21	5:E:214:ILE:HD13	1.90	0.53
3:H:120:GLU:N	3:H:121:GLY:HA3	2.23	0.53
3:W:120:GLU:N	3:W:121:GLY:HA3	2.22	0.53
5:4:221:GLY:C	5:4:223:LEU:N	2.61	0.53
1:F:83:LEU:HD11	7:F:201:HEM:HMA1	1.90	0.53
3:W:128:ASN:HB3	3:W:130:GLU:N	2.23	0.53
3:W:130:GLU:N	3:W:130:GLU:OE1	2.41	0.53
1:Z:44:PRO:HB2	1:Z:45:HIS:ND1	2.23	0.53
2:B:122:PHE:CE2	2:B:127:GLN:HB2	2.44	0.53
5:J:126:THR:O	5:J:130:GLU:HG2	2.09	0.53
4:S:194:GLN:HG3	4:S:222:PRO:HA	1.91	0.53
5:T:226:HIS:O	5:T:229:LYS:HG2	2.08	0.53
1:Z:3:SER:N	1:Z:6:ASP:OD2	2.38	0.53
4:3:198:ILE:HB	4:3:215:THR:HB	1.91	0.53
4:N:158:LYS:O	4:N:200:SER:HA	2.09	0.53
5:O:206:SER:HB3	5:O:208:THR:H	1.73	0.53
3:R:151:LYS:H	3:R:259:MET:CE	2.22	0.53
3:W:221:VAL:HG23	3:W:225:GLN:HB3	1.90	0.53
5:4:47:LYS:HD3	5:4:216:ALA:O	2.08	0.53
3:C:162:HIS:HB3	3:C:294:TYR:CE2	2.43	0.53
5:O:221:GLY:C	5:O:223:LEU:N	2.62	0.53
1:P:3:SER:N	1:P:6:ASP:OD2	2.37	0.53
3:2:120:GLU:N	3:2:121:GLY:HA3	2.23	0.53
3:M:120:GLU:N	3:M:121:GLY:HA3	2.23	0.53
3:R:254:VAL:HG13	3:R:259:MET:HB2	1.90	0.53
1:Z:92:ARG:NH1	1:Z:141:ARG:O	2.41	0.53
5:4:126:THR:O	5:4:130:GLU:HG2	2.09	0.53
3:H:336:CYS:SG	3:H:384:VAL:HG23	2.49	0.52
5:E:221:GLY:C	5:E:223:LEU:N	2.62	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:122:PHE:CE2	2:L:127:GLN:HB2	2.44	0.52
3:C:128:ASN:HB3	3:C:130:GLU:N	2.24	0.52
3:H:186:THR:HG23	3:H:352:GLY:O	2.09	0.52
5:4:43:ASP:OD2	5:4:47:LYS:HE2	2.09	0.52
3:2:254:VAL:HG13	3:2:259:MET:HB2	1.91	0.52
3:R:196:THR:OG1	3:R:199:ASN:OD1	2.19	0.52
1:U:98:PHE:HB3	1:U:133:SER:OG	2.09	0.52
2:V:19:ASN:ND2	2:V:22:GLU:HB2	2.25	0.52
1:A:129:LEU:O	1:A:133:SER:HB2	2.10	0.52
5:E:226:HIS:O	5:E:229:LYS:HG2	2.10	0.52
1:F:11:LYS:NZ	4:I:151:ASN:OD1	2.38	0.52
3:H:374:ASP:OD1	3:H:374:ASP:N	2.30	0.52
5:T:38:GLY:HA3	5:T:177:LEU:HG	1.91	0.52
5:T:191:LYS:NZ	5:T:195:GLU:OE2	2.42	0.52
3:2:271:VAL:HA	3:2:299:VAL:HG22	1.91	0.52
3:C:120:GLU:N	3:C:121:GLY:HA3	2.24	0.52
1:U:44:PRO:HB2	1:U:45:HIS:ND1	2.24	0.52
3:C:188:ILE:HG12	3:C:263:LEU:HD11	1.92	0.52
2:L:24:GLY:N	2:L:68:LEU:HD22	2.22	0.52
4:X:158:LYS:O	4:X:200:SER:HA	2.10	0.52
5:4:166:LYS:HB3	5:4:233:VAL:HG12	1.91	0.52
1:F:107:VAL:HG11	2:G:127:GLN:OE1	2.09	0.51
7:F:201:HEM:HMB1	7:F:201:HEM:HBB2	1.92	0.51
3:H:340:SER:HB3	3:H:344:GLU:H	1.75	0.51
3:H:340:SER:HB3	3:H:344:GLU:N	2.25	0.51
1:K:17:VAL:HG13	1:K:24:TYR:CD1	2.45	0.51
3:R:302:GLN:O	3:R:306:ILE:HG12	2.09	0.51
3:W:373:PHE:CB	3:W:384:VAL:HG12	2.35	0.51
5:Y:43:ASP:OD2	5:Y:47:LYS:HE2	2.10	0.51
2:B:24:GLY:N	2:B:68:LEU:HD22	2.22	0.51
3:M:151:LYS:H	3:M:259:MET:HE2	1.75	0.51
4:S:94:ILE:HD12	4:S:175:TYR:CZ	2.45	0.51
4:D:194:GLN:HG3	4:D:222:PRO:HA	1.91	0.51
3:H:306:ILE:HD13	3:H:330:LEU:HD13	1.90	0.51
5:J:65:ILE:HG22	5:J:244:VAL:HG21	1.93	0.51
4:N:198:ILE:HB	4:N:215:THR:HB	1.92	0.51
1:P:6:ASP:O	1:P:10:VAL:HG23	2.10	0.51
5:4:108:LYS:HA	5:4:112:LYS:HG2	1.92	0.51
3:C:96:PRO:HG2	3:H:142:LEU:HD11	1.93	0.51
4:I:198:ILE:HB	4:I:215:THR:HB	1.93	0.51
5:Y:65:ILE:HG22	5:Y:244:VAL:HG21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:162:HIS:HB3	3:2:294:TYR:CE2	2.45	0.51
5:4:38:GLY:HA3	5:4:177:LEU:HG	1.91	0.51
1:K:129:LEU:O	1:K:133:SER:HB2	2.11	0.51
1:U:84:SER:HB3	1:U:139:LYS:HD2	1.93	0.51
5:Y:38:GLY:HA3	5:Y:177:LEU:HG	1.92	0.51
3:2:306:ILE:HD13	3:2:330:LEU:HD13	1.91	0.51
3:2:340:SER:HB3	3:2:344:GLU:H	1.75	0.51
3:R:271:VAL:HA	3:R:299:VAL:HG22	1.92	0.51
3:R:340:SER:HB3	3:R:344:GLU:H	1.75	0.51
3:2:151:LYS:H	3:2:259:MET:HE1	1.74	0.51
4:3:158:LYS:O	4:3:200:SER:HA	2.10	0.51
5:E:108:LYS:HA	5:E:112:LYS:HG2	1.91	0.51
4:I:194:GLN:HG3	4:I:222:PRO:HA	1.93	0.51
2:L:18:VAL:HG13	2:L:23:VAL:HG21	1.93	0.51
3:M:303:ASP:HB3	3:M:307:ARG:NH2	2.26	0.51
3:R:119:THR:CG2	3:R:143:PRO:HB3	2.41	0.51
3:R:345:ASP:OD1	3:R:346:THR:HG22	2.11	0.51
4:X:194:GLN:HG3	4:X:222:PRO:HA	1.91	0.51
1:K:11:LYS:NZ	4:N:151:ASN:OD1	2.43	0.51
5:T:97:LEU:HD21	5:T:129:ARG:HE	1.76	0.51
5:4:191:LYS:NZ	5:4:195:GLU:OE2	2.44	0.51
5:4:226:HIS:O	5:4:229:LYS:HG2	2.10	0.51
4:D:113:ASN:ND2	5:O:202:SER:OG	2.44	0.51
5:O:42:LYS:HG3	5:O:193:ALA:HB2	1.93	0.51
3:R:340:SER:HB3	3:R:344:GLU:N	2.26	0.51
3:C:142:LEU:HD11	3:H:96:PRO:CG	2.42	0.50
3:C:221:VAL:HG23	3:C:225:GLN:HB3	1.91	0.50
5:E:42:LYS:HG3	5:E:193:ALA:HB2	1.93	0.50
5:J:38:GLY:HA3	5:J:177:LEU:HG	1.92	0.50
3:M:271:VAL:HA	3:M:299:VAL:HG22	1.93	0.50
5:O:108:LYS:HA	5:O:112:LYS:HG2	1.92	0.50
5:T:49:CYS:HA	5:T:178:LEU:HD21	1.93	0.50
3:W:145:CYS:HB2	3:2:99:ALA:O	2.11	0.50
1:F:35:SER:HB3	2:G:131:GLN:HG3	1.94	0.50
5:O:43:ASP:OD2	5:O:47:LYS:HE2	2.12	0.50
4:S:158:LYS:O	4:S:200:SER:HA	2.11	0.50
3:2:162:HIS:HB2	3:2:294:TYR:O	2.10	0.50
5:4:49:CYS:HA	5:4:178:LEU:HD21	1.93	0.50
3:C:119:THR:CG2	3:C:143:PRO:HB3	2.41	0.50
3:M:306:ILE:HD13	3:M:330:LEU:HD13	1.92	0.50
3:M:321:LYS:O	3:M:323:PRO:HD3	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:129:LEU:O	1:U:133:SER:HB2	2.12	0.50
3:W:302:GLN:O	3:W:306:ILE:HG12	2.11	0.50
2:1:24:GLY:N	2:1:68:LEU:HD22	2.22	0.50
2:G:97:HIS:HB3	3:H:163:LEU:HD12	1.93	0.50
3:M:255:ASN:OD1	3:M:257:ARG:HG2	2.11	0.50
4:N:194:GLN:HG3	4:N:222:PRO:HA	1.92	0.50
5:O:191:LYS:NZ	5:O:195:GLU:OE2	2.44	0.50
2:1:122:PHE:CE2	2:1:127:GLN:HB2	2.46	0.50
2:B:109:VAL:O	2:B:113:VAL:HG23	2.11	0.50
5:E:127:SER:HA	5:E:130:GLU:HG2	1.94	0.50
5:J:166:LYS:HB3	5:J:233:VAL:HG12	1.93	0.50
3:M:340:SER:HB3	3:M:344:GLU:H	1.75	0.50
5:Y:226:HIS:O	5:Y:229:LYS:HG2	2.12	0.50
5:Y:287:ASN:O	5:Y:291:THR:OG1	2.18	0.50
2:1:106:LEU:HD23	7:1:201:HEM:CBB	2.42	0.50
4:3:131:ILE:HG21	4:3:148:LEU:HD22	1.93	0.50
4:D:198:ILE:HB	4:D:215:THR:HB	1.93	0.50
5:Y:206:SER:HB3	5:Y:208:THR:H	1.76	0.50
3:H:188:ILE:HG12	3:H:263:LEU:HD11	1.94	0.50
5:J:43:ASP:OD2	5:J:47:LYS:HE2	2.11	0.50
3:M:223:LYS:HD3	3:M:257:ARG:NH1	2.26	0.50
5:T:43:ASP:OD2	5:T:47:LYS:HE2	2.11	0.50
1:A:17:VAL:HG13	1:A:24:TYR:CD1	2.46	0.50
2:G:24:GLY:N	2:G:68:LEU:HD22	2.23	0.50
3:R:264:PRO:HB2	3:R:266:LYS:O	2.12	0.50
3:W:186:THR:HG23	3:W:352:GLY:O	2.12	0.50
4:3:87:ASP:HB2	4:3:159:PHE:O	2.12	0.50
3:H:223:LYS:HD3	3:H:257:ARG:NH1	2.26	0.50
5:J:97:LEU:HD21	5:J:129:ARG:HE	1.77	0.50
5:O:38:GLY:HA3	5:O:177:LEU:HG	1.93	0.50
4:S:87:ASP:HB2	4:S:159:PHE:O	2.12	0.50
2:V:123:THR:OG1	2:V:125:PRO:HD2	2.12	0.50
2:B:18:VAL:HG13	2:B:23:VAL:HG21	1.94	0.49
3:C:321:LYS:O	3:C:323:PRO:HD3	2.12	0.49
3:H:119:THR:CG2	3:H:143:PRO:HB3	2.42	0.49
4:I:87:ASP:HB2	4:I:159:PHE:O	2.12	0.49
4:S:198:ILE:HB	4:S:215:THR:HB	1.94	0.49
3:W:162:HIS:HB3	3:W:294:TYR:CE2	2.46	0.49
4:X:198:ILE:HB	4:X:215:THR:HB	1.93	0.49
5:4:56:LYS:NZ	5:4:59:SER:OG	2.44	0.49
3:C:337:ALA:HB3	3:C:385:TYR:HE1	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:75:LEU:HD21	2:G:133:VAL:HG11	1.94	0.49
3:2:350:ASP:O	3:2:371:LEU:HD12	2.12	0.49
2:B:123:THR:OG1	2:B:125:PRO:HD2	2.13	0.49
3:C:114:TYR:O	3:C:148:VAL:HG23	2.12	0.49
5:E:38:GLY:HA3	5:E:177:LEU:HG	1.94	0.49
2:L:123:THR:OG1	2:L:125:PRO:HD2	2.12	0.49
3:M:340:SER:HB3	3:M:344:GLU:N	2.27	0.49
2:Q:75:LEU:HD21	2:Q:133:VAL:HG11	1.94	0.49
1:Z:129:LEU:O	1:Z:133:SER:HB2	2.12	0.49
3:C:296:MET:CE	5:E:71:ARG:HA	2.42	0.49
4:N:87:ASP:HB2	4:N:159:PHE:O	2.11	0.49
3:R:170:PRO:HB2	3:R:259:MET:HG2	1.94	0.49
3:R:238:TYR:CD1	3:R:238:TYR:N	2.81	0.49
3:R:324:VAL:HG23	3:R:326:VAL:H	1.76	0.49
3:C:109:TYR:OH	3:H:96:PRO:O	2.16	0.49
4:D:94:ILE:HD12	4:D:175:TYR:CZ	2.47	0.49
5:J:49:CYS:HA	5:J:178:LEU:HD21	1.94	0.49
3:M:388:VAL:O	3:M:391:ILE:HG13	2.13	0.49
3:2:324:VAL:HG23	3:2:326:VAL:H	1.77	0.49
5:4:97:LEU:HD21	5:4:129:ARG:HE	1.77	0.49
3:M:196:THR:HG21	3:M:351:ALA:HB1	1.95	0.49
1:P:107:VAL:HG11	2:Q:127:GLN:OE1	2.11	0.49
3:W:306:ILE:HD13	3:W:330:LEU:HD13	1.93	0.49
5:J:42:LYS:HG3	5:J:193:ALA:HB2	1.95	0.49
4:S:96:ASP:HB3	4:S:99:LEU:HD22	1.95	0.49
3:W:156:ALA:O	3:W:157:ASN:HB2	2.13	0.49
1:Z:83:LEU:HD11	7:Z:201:HEM:HMA1	1.94	0.49
3:2:119:THR:CG2	3:2:143:PRO:HB3	2.43	0.49
5:J:44:GLU:CD	5:J:221:GLY:HA3	2.33	0.49
1:Z:6:ASP:O	1:Z:10:VAL:HG23	2.12	0.49
1:Z:17:VAL:HG13	1:Z:24:TYR:CD1	2.47	0.49
3:C:114:TYR:CD2	3:C:255:ASN:HA	2.47	0.49
3:M:170:PRO:HB2	3:M:259:MET:HG2	1.95	0.49
3:W:255:ASN:OD1	3:W:257:ARG:HG2	2.12	0.49
3:W:271:VAL:HA	3:W:299:VAL:HG22	1.94	0.49
3:2:340:SER:HB3	3:2:344:GLU:N	2.28	0.49
5:4:42:LYS:HG3	5:4:193:ALA:HB2	1.95	0.49
3:H:350:ASP:C	3:H:371:LEU:HD12	2.34	0.49
4:I:94:ILE:HD12	4:I:175:TYR:CZ	2.47	0.49
4:N:145:GLU:OE2	4:N:171:ARG:NH2	2.40	0.49
3:C:303:ASP:HB3	3:C:307:ARG:NH2	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:153:LYS:HB3	3:H:256:GLU:HB2	1.94	0.48
3:M:143:PRO:HG2	3:R:98:ILE:HD13	1.95	0.48
3:W:119:THR:CG2	3:W:143:PRO:HB3	2.43	0.48
5:Y:97:LEU:HD21	5:Y:129:ARG:HE	1.77	0.48
4:I:158:LYS:O	4:I:200:SER:HA	2.12	0.48
2:Q:123:THR:OG1	2:Q:125:PRO:HD2	2.13	0.48
1:U:6:ASP:O	1:U:10:VAL:HG23	2.12	0.48
2:V:63:HIS:O	2:V:67:VAL:HG23	2.13	0.48
3:W:350:ASP:O	3:W:371:LEU:HD12	2.13	0.48
4:X:96:ASP:HB3	4:X:99:LEU:HD22	1.96	0.48
2:1:75:LEU:HD21	2:1:133:VAL:HG11	1.95	0.48
3:2:156:ALA:O	3:2:157:ASN:HB2	2.13	0.48
4:D:87:ASP:HB2	4:D:159:PHE:O	2.12	0.48
2:G:123:THR:OG1	2:G:125:PRO:HD2	2.13	0.48
3:H:162:HIS:HB3	3:H:294:TYR:CE2	2.48	0.48
1:K:66:LEU:O	1:K:70:VAL:HG12	2.14	0.48
1:K:107:VAL:HG11	2:L:127:GLN:OE1	2.13	0.48
3:M:107:VAL:HG11	3:R:95:PRO:HG3	1.95	0.48
3:R:114:TYR:CD2	3:R:255:ASN:HA	2.48	0.48
3:R:188:ILE:HG12	3:R:263:LEU:HD11	1.95	0.48
5:T:44:GLU:CD	5:T:221:GLY:HA3	2.33	0.48
3:W:142:LEU:HD11	3:2:96:PRO:CG	2.44	0.48
4:D:145:GLU:OE2	4:D:171:ARG:NH2	2.41	0.48
4:I:126:TYR:CE2	4:I:202:THR:HG21	2.48	0.48
3:R:340:SER:OG	3:R:341:LYS:N	2.45	0.48
4:3:96:ASP:HB3	4:3:99:LEU:HD22	1.96	0.48
3:C:196:THR:HG21	3:C:351:ALA:HB1	1.95	0.48
4:D:96:ASP:HB3	4:D:99:LEU:HD22	1.96	0.48
3:H:321:LYS:O	3:H:323:PRO:HD3	2.13	0.48
3:H:324:VAL:HG23	3:H:326:VAL:H	1.78	0.48
5:J:256:LYS:HE3	5:J:260:LYS:HE3	1.96	0.48
3:M:119:THR:CG2	3:M:143:PRO:HB3	2.43	0.48
3:R:374:ASP:OD1	3:R:374:ASP:N	2.35	0.48
4:S:131:ILE:HG21	4:S:148:LEU:HD22	1.95	0.48
5:T:42:LYS:HG3	5:T:193:ALA:HB2	1.96	0.48
3:W:119:THR:HG21	3:W:143:PRO:HB3	1.95	0.48
5:Y:191:LYS:NZ	5:Y:195:GLU:OE2	2.44	0.48
5:E:121:ILE:O	5:E:125:ILE:HG12	2.13	0.48
3:H:135:ASN:O	3:H:139:GLY:N	2.43	0.48
4:I:131:ILE:HG21	4:I:148:LEU:HD22	1.94	0.48
3:M:162:HIS:HB2	3:M:294:TYR:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:88:LEU:HD21	7:V:201:HEM:HMA3	1.95	0.48
4:3:126:TYR:CE2	4:3:202:THR:HG21	2.48	0.48
3:C:162:HIS:HB2	3:C:294:TYR:O	2.13	0.48
3:C:223:LYS:HD3	3:C:257:ARG:NH1	2.28	0.48
2:G:109:VAL:O	2:G:113:VAL:HG23	2.14	0.48
3:H:302:GLN:O	3:H:306:ILE:HG12	2.12	0.48
3:H:345:ASP:OD1	3:H:346:THR:HG22	2.14	0.48
3:M:238:TYR:N	3:M:238:TYR:CD1	2.82	0.48
5:O:39:LEU:HD23	5:O:40:LYS:H	1.79	0.48
2:Q:88:LEU:O	2:Q:92:HIS:ND1	2.42	0.48
3:W:183:THR:HB	3:W:199:ASN:ND2	2.19	0.48
5:Y:49:CYS:HA	5:Y:178:LEU:HD21	1.94	0.48
3:C:238:TYR:CD1	3:C:238:TYR:N	2.82	0.48
3:C:271:VAL:HA	3:C:299:VAL:HG22	1.96	0.48
4:I:96:ASP:HB3	4:I:99:LEU:HD22	1.96	0.48
5:O:49:CYS:HA	5:O:178:LEU:HD21	1.94	0.48
2:Q:109:VAL:O	2:Q:113:VAL:HG23	2.14	0.48
4:3:145:GLU:OE2	4:3:171:ARG:NH2	2.41	0.48
3:C:198:LYS:NZ	3:C:329:ILE:HD11	2.29	0.48
3:C:336:CYS:SG	3:C:384:VAL:HG23	2.53	0.48
1:F:17:VAL:HG13	1:F:24:TYR:CD1	2.48	0.48
1:K:9:ASN:ND2	1:K:121:VAL:HG22	2.24	0.48
3:R:162:HIS:HB3	3:R:294:TYR:CE2	2.49	0.48
3:R:336:CYS:SG	3:R:384:VAL:HG23	2.54	0.48
3:2:186:THR:HG23	3:2:352:GLY:O	2.13	0.48
5:E:44:GLU:CD	5:E:221:GLY:HA3	2.34	0.48
2:G:31:LEU:HD13	2:G:106:LEU:HB2	1.95	0.48
3:M:183:THR:HB	3:M:199:ASN:ND2	2.17	0.48
3:R:350:ASP:C	3:R:371:LEU:HD12	2.35	0.48
4:D:131:ILE:HG21	4:D:148:LEU:HD22	1.96	0.47
3:M:374:ASP:OD1	3:M:374:ASP:N	2.28	0.47
7:Q:201:HEM:HHD	7:Q:201:HEM:CBC	2.44	0.47
1:U:17:VAL:HG13	1:U:24:TYR:CD1	2.49	0.47
5:Y:44:GLU:CD	5:Y:221:GLY:HA3	2.35	0.47
3:H:238:TYR:CD1	3:H:238:TYR:N	2.83	0.47
5:J:38:GLY:O	5:J:39:LEU:HB2	2.14	0.47
3:M:153:LYS:HB3	3:M:256:GLU:HB2	1.96	0.47
5:O:44:GLU:CD	5:O:221:GLY:HA3	2.35	0.47
3:R:223:LYS:HD3	3:R:257:ARG:NH1	2.28	0.47
1:U:107:VAL:HG11	2:V:127:GLN:OE1	2.14	0.47
5:Y:43:ASP:O	5:Y:46:GLU:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:LYS:H	3:C:259:MET:HE2	1.79	0.47
3:C:340:SER:HB3	3:C:344:GLU:H	1.78	0.47
3:C:340:SER:HB3	3:C:344:GLU:N	2.29	0.47
3:M:160:GLY:HA3	3:M:344:GLU:HG2	1.96	0.47
3:R:119:THR:HG21	3:R:143:PRO:HB3	1.96	0.47
3:R:153:LYS:HB3	3:R:256:GLU:HB2	1.96	0.47
3:R:306:ILE:HD13	3:R:330:LEU:HD13	1.94	0.47
3:W:337:ALA:HB3	3:W:385:TYR:HE1	1.78	0.47
5:Y:51:LEU:HA	5:Y:51:LEU:HD23	1.72	0.47
5:Y:121:ILE:O	5:Y:125:ILE:HG12	2.14	0.47
3:M:302:GLN:O	3:M:306:ILE:HG12	2.14	0.47
3:R:151:LYS:H	3:R:259:MET:HE1	1.79	0.47
4:S:126:TYR:CE2	4:S:202:THR:HG21	2.49	0.47
4:X:87:ASP:HB2	4:X:159:PHE:O	2.13	0.47
4:X:131:ILE:HG21	4:X:148:LEU:HD22	1.96	0.47
5:Y:42:LYS:HG3	5:Y:193:ALA:HB2	1.96	0.47
3:2:188:ILE:HG12	3:2:263:LEU:HD11	1.96	0.47
3:C:119:THR:HG21	3:C:143:PRO:HB3	1.96	0.47
3:H:170:PRO:HB2	3:H:259:MET:HG2	1.96	0.47
2:L:51:PRO:O	2:L:55:MET:HG2	2.15	0.47
3:W:151:LYS:H	3:W:259:MET:HE2	1.79	0.47
2:1:63:HIS:O	2:1:67:VAL:HG23	2.15	0.47
3:2:238:TYR:CD1	3:2:238:TYR:N	2.83	0.47
3:C:135:ASN:O	3:C:139:GLY:N	2.43	0.47
1:F:6:ASP:O	1:F:10:VAL:HG23	2.13	0.47
2:L:41:PHE:HB3	7:L:201:HEM:HMD2	1.97	0.47
5:T:43:ASP:O	5:T:46:GLU:HG2	2.15	0.47
3:2:337:ALA:HB3	3:2:385:TYR:HE1	1.79	0.47
3:C:156:ALA:O	3:C:157:ASN:HB2	2.14	0.47
3:C:170:PRO:HB2	3:C:259:MET:HG2	1.97	0.47
3:C:302:GLN:O	3:C:306:ILE:HG12	2.14	0.47
3:C:388:VAL:O	3:C:391:ILE:HG13	2.15	0.47
5:E:39:LEU:HD23	5:E:40:LYS:H	1.80	0.47
3:M:174:LYS:HB2	3:M:280:TRP:CG	2.49	0.47
3:M:198:LYS:NZ	3:M:329:ILE:HD11	2.30	0.47
2:Q:24:GLY:N	2:Q:68:LEU:HD22	2.26	0.47
3:W:175:MET:HB2	3:W:219:LEU:HD13	1.95	0.47
3:W:324:VAL:HG23	3:W:326:VAL:H	1.78	0.47
3:2:119:THR:HG21	3:2:143:PRO:HB3	1.97	0.47
3:H:92:CYS:SG	3:H:92:CYS:O	2.72	0.47
1:K:6:ASP:O	1:K:10:VAL:HG23	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:245:LEU:HD23	3:R:245:LEU:HA	1.62	0.47
2:V:109:VAL:O	2:V:113:VAL:HG23	2.15	0.47
3:W:162:HIS:HB2	3:W:294:TYR:O	2.15	0.47
3:W:238:TYR:N	3:W:238:TYR:CD1	2.83	0.47
3:2:223:LYS:HD3	3:2:257:ARG:NH1	2.29	0.47
3:2:321:LYS:O	3:2:323:PRO:HD3	2.14	0.47
3:C:153:LYS:HB3	3:C:256:GLU:HB2	1.96	0.47
3:C:296:MET:HE1	5:E:71:ARG:HA	1.97	0.47
3:C:374:ASP:OD1	3:C:374:ASP:N	2.29	0.47
4:D:126:TYR:CE2	4:D:202:THR:HG21	2.50	0.47
3:H:245:LEU:HD23	3:H:245:LEU:HA	1.64	0.47
3:M:188:ILE:CG1	3:M:263:LEU:HD11	2.44	0.47
3:M:224:LYS:HB3	3:M:224:LYS:HE2	1.76	0.47
5:O:121:ILE:O	5:O:125:ILE:HG12	2.14	0.47
3:R:303:ASP:HB3	3:R:307:ARG:NH2	2.29	0.47
3:W:312:SER:HB2	3:W:314:VAL:O	2.15	0.47
3:W:345:ASP:OD1	3:W:346:THR:HG22	2.15	0.47
1:A:11:LYS:NZ	4:D:151:ASN:OD1	2.47	0.47
1:A:66:LEU:O	1:A:70:VAL:HG12	2.15	0.47
5:E:97:LEU:HD21	5:E:129:ARG:HE	1.79	0.47
3:H:119:THR:HG21	3:H:143:PRO:HB3	1.97	0.47
3:M:184:GLY:O	3:M:352:GLY:HA3	2.15	0.47
3:R:388:VAL:O	3:R:391:ILE:HG13	2.14	0.47
3:W:223:LYS:HD3	3:W:257:ARG:NH1	2.29	0.47
4:X:94:ILE:HD12	4:X:175:TYR:CZ	2.50	0.47
3:2:374:ASP:OD1	3:2:374:ASP:N	2.37	0.47
2:B:71:PHE:CE2	2:B:137:VAL:HG11	2.50	0.46
2:L:101:GLU:OE1	2:L:101:GLU:HA	2.16	0.46
4:N:126:TYR:CE2	4:N:202:THR:HG21	2.50	0.46
2:Q:63:HIS:O	2:Q:67:VAL:HG23	2.15	0.46
3:R:314:VAL:HA	3:R:315:PRO:HD3	1.80	0.46
2:1:123:THR:OG1	2:1:125:PRO:HD2	2.15	0.46
1:A:3:SER:N	1:A:6:ASP:OD2	2.39	0.46
3:C:224:LYS:HB3	3:C:224:LYS:HE2	1.76	0.46
3:H:388:VAL:O	3:H:391:ILE:HG13	2.15	0.46
1:P:129:LEU:O	1:P:133:SER:HB2	2.15	0.46
3:R:321:LYS:O	3:R:323:PRO:HD3	2.15	0.46
3:W:114:TYR:CD2	3:W:255:ASN:HA	2.50	0.46
5:4:44:GLU:CD	5:4:221:GLY:HA3	2.35	0.46
5:J:46:GLU:HA	5:J:49:CYS:HB3	1.97	0.46
5:O:97:LEU:HD21	5:O:129:ARG:HE	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:38:GLY:O	5:T:39:LEU:HB2	2.15	0.46
1:Z:48:LEU:HD23	1:Z:48:LEU:HA	1.73	0.46
1:Z:119:PRO:HG2	2:1:55:MET:HG3	1.97	0.46
5:4:38:GLY:O	5:4:39:LEU:HB2	2.15	0.46
5:E:173:ASP:OD2	5:E:229:LYS:NZ	2.48	0.46
3:M:119:THR:HG23	3:M:121:GLY:CA	2.45	0.46
3:M:277:VAL:HG12	3:M:278:SER:O	2.16	0.46
3:M:306:ILE:CD1	3:M:330:LEU:HD13	2.46	0.46
4:N:94:ILE:HD12	4:N:175:TYR:CZ	2.50	0.46
1:P:14:TRP:HE1	1:P:67:THR:HG23	1.80	0.46
5:T:46:GLU:HA	5:T:49:CYS:HB3	1.97	0.46
1:U:27:GLU:OE2	1:U:108:THR:HG23	2.16	0.46
3:2:153:LYS:HB3	3:2:256:GLU:HB2	1.97	0.46
5:4:121:ILE:O	5:4:125:ILE:HG12	2.14	0.46
3:C:376:SER:HB2	3:C:380:ALA:O	2.15	0.46
4:N:140:THR:OG1	4:N:143:LYS:O	2.32	0.46
5:O:166:LYS:HD2	5:O:232:ASP:HB2	1.98	0.46
1:P:17:VAL:HG13	1:P:24:TYR:CD1	2.50	0.46
5:T:121:ILE:O	5:T:125:ILE:HG12	2.14	0.46
3:W:188:ILE:HG12	3:W:263:LEU:HD11	1.97	0.46
9:4:1002:NAG:HO3	9:4:1002:NAG:C7	2.24	0.46
1:A:14:TRP:HE1	1:A:67:THR:HG23	1.81	0.46
3:H:306:ILE:CD1	3:H:330:LEU:HD13	2.45	0.46
3:M:135:ASN:O	3:M:139:GLY:N	2.44	0.46
2:Q:71:PHE:CE2	2:Q:137:VAL:HG11	2.50	0.46
3:R:196:THR:HG21	3:R:351:ALA:HB1	1.97	0.46
3:W:321:LYS:O	3:W:323:PRO:HD3	2.15	0.46
1:Z:65:ALA:HB2	7:Z:201:HEM:HMA1	1.98	0.46
3:2:245:LEU:HD23	3:2:245:LEU:HA	1.63	0.46
2:B:142:ALA:O	2:B:145:TYR:HB2	2.15	0.46
3:H:303:ASP:HB3	3:H:307:ARG:NH2	2.30	0.46
3:M:324:VAL:HG23	3:M:326:VAL:H	1.80	0.46
4:3:94:ILE:HD12	4:3:175:TYR:CZ	2.50	0.46
2:B:75:LEU:HD21	2:B:133:VAL:HG11	1.97	0.46
3:C:255:ASN:OD1	3:C:257:ARG:HG2	2.15	0.46
3:C:306:ILE:HD13	3:C:330:LEU:HD13	1.97	0.46
3:M:350:ASP:C	3:M:371:LEU:HD12	2.36	0.46
3:W:186:THR:HG21	3:W:354:ALA:CB	2.45	0.46
5:Y:61:THR:O	5:Y:65:ILE:HG13	2.15	0.46
5:J:121:ILE:O	5:J:125:ILE:HG12	2.15	0.46
3:M:96:PRO:HG2	3:R:142:LEU:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:43:ASP:O	5:O:46:GLU:HG2	2.16	0.46
5:O:51:LEU:HD23	5:O:51:LEU:HA	1.76	0.46
2:V:142:ALA:O	2:V:145:TYR:HB2	2.16	0.46
3:C:183:THR:HB	3:C:199:ASN:ND2	2.20	0.46
2:V:18:VAL:HG13	2:V:23:VAL:HG21	1.98	0.46
2:B:92:HIS:HA	2:B:96:LEU:HB2	1.97	0.45
3:C:277:VAL:HG12	3:C:278:SER:O	2.17	0.45
3:C:314:VAL:HA	3:C:315:PRO:HD3	1.75	0.45
5:E:49:CYS:HA	5:E:178:LEU:HD21	1.97	0.45
2:L:118:PHE:O	2:L:121:GLU:HB3	2.16	0.45
3:W:96:PRO:HG2	3:2:142:LEU:HD11	1.96	0.45
3:2:198:LYS:NZ	3:2:329:ILE:HD11	2.31	0.45
3:M:114:TYR:CD2	3:M:255:ASN:HA	2.51	0.45
3:W:198:LYS:NZ	3:W:329:ILE:HD11	2.31	0.45
3:W:303:ASP:HB3	3:W:307:ARG:NH2	2.31	0.45
5:J:43:ASP:O	5:J:46:GLU:HG2	2.17	0.45
3:M:373:PHE:CZ	3:M:375:LYS:HB2	2.52	0.45
3:M:376:SER:HB2	3:M:380:ALA:O	2.16	0.45
1:P:48:LEU:HD23	1:P:48:LEU:HA	1.75	0.45
1:P:83:LEU:HD11	7:P:201:HEM:HMA1	1.97	0.45
1:U:9:ASN:ND2	1:U:121:VAL:HG22	2.26	0.45
2:V:75:LEU:HD21	2:V:133:VAL:HG11	1.98	0.45
3:C:128:ASN:HD22	3:C:130:GLU:HB2	1.80	0.45
3:C:373:PHE:CZ	3:C:375:LYS:HB2	2.51	0.45
5:E:51:LEU:HD23	5:E:51:LEU:HA	1.76	0.45
1:F:48:LEU:HD23	1:F:48:LEU:HA	1.76	0.45
5:J:44:GLU:OE2	5:J:221:GLY:HA3	2.17	0.45
1:K:106:LEU:HD23	1:K:106:LEU:HA	1.82	0.45
3:M:314:VAL:HA	3:M:315:PRO:HD3	1.76	0.45
5:T:39:LEU:HD23	5:T:40:LYS:H	1.81	0.45
5:Y:38:GLY:O	5:Y:39:LEU:HB2	2.17	0.45
1:Z:27:GLU:OE2	1:Z:108:THR:HG23	2.17	0.45
5:4:39:LEU:HD23	5:4:40:LYS:H	1.81	0.45
2:G:69:GLY:O	2:G:72:SER:N	2.50	0.45
4:I:140:THR:OG1	4:I:143:LYS:O	2.31	0.45
2:1:8:LYS:O	2:1:12:THR:OG1	2.29	0.45
3:2:184:GLY:O	3:2:352:GLY:HA3	2.15	0.45
5:J:39:LEU:HD23	5:J:40:LYS:H	1.81	0.45
2:L:92:HIS:HA	2:L:96:LEU:HB2	1.98	0.45
2:L:109:VAL:O	2:L:113:VAL:HG23	2.17	0.45
5:O:38:GLY:O	5:O:39:LEU:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:97:HIS:HB3	3:R:163:LEU:HD12	1.98	0.45
3:W:336:CYS:SG	3:W:384:VAL:HG23	2.57	0.45
4:X:126:TYR:CE2	4:X:202:THR:HG21	2.51	0.45
3:2:135:ASN:O	3:2:139:GLY:N	2.46	0.45
3:2:303:ASP:HB3	3:2:307:ARG:NH2	2.31	0.45
2:L:75:LEU:HD21	2:L:133:VAL:HG11	1.98	0.45
3:M:334:THR:HA	3:M:386:VAL:HA	1.99	0.45
3:R:92:CYS:O	3:R:92:CYS:SG	2.74	0.45
5:E:191:LYS:NZ	5:E:195:GLU:OE2	2.48	0.45
3:H:114:TYR:CD2	3:H:255:ASN:HA	2.51	0.45
3:H:118:ARG:O	3:H:119:THR:HB	2.17	0.45
2:L:142:ALA:O	2:L:145:TYR:HB2	2.17	0.45
3:M:119:THR:HG21	3:M:143:PRO:HB3	1.98	0.45
3:M:312:SER:HB2	3:M:314:VAL:O	2.17	0.45
3:R:135:ASN:O	3:R:139:GLY:N	2.45	0.45
3:R:391:ILE:O	3:R:395:VAL:HG22	2.17	0.45
3:W:153:LYS:HB3	3:W:256:GLU:HB2	1.98	0.45
3:2:302:GLN:O	3:2:306:ILE:HG12	2.16	0.45
5:4:126:THR:HG23	5:4:127:SER:H	1.82	0.45
1:A:107:VAL:HG11	2:B:127:GLN:OE1	2.17	0.45
1:F:99:LYS:HA	1:F:99:LYS:HD3	1.40	0.45
3:H:312:SER:HB2	3:H:314:VAL:O	2.16	0.45
5:J:287:ASN:O	5:J:291:THR:OG1	2.18	0.45
7:L:201:HEM:HHD	7:L:201:HEM:CBC	2.46	0.45
3:M:186:THR:HG21	3:M:354:ALA:CB	2.46	0.45
2:Q:142:ALA:O	2:Q:145:TYR:HB2	2.17	0.45
2:B:98:VAL:O	2:B:145:TYR:OH	2.23	0.45
5:T:287:ASN:O	5:T:291:THR:OG1	2.19	0.45
1:U:11:LYS:NZ	4:X:151:ASN:OD1	2.49	0.45
3:W:170:PRO:HB2	3:W:259:MET:HG2	1.99	0.45
3:2:312:SER:HB2	3:2:314:VAL:O	2.16	0.45
2:B:51:PRO:O	2:B:55:MET:HG2	2.17	0.44
3:C:119:THR:HG23	3:C:121:GLY:CA	2.46	0.44
3:H:188:ILE:CG1	3:H:263:LEU:HD11	2.47	0.44
2:L:71:PHE:CE2	2:L:137:VAL:HG11	2.52	0.44
4:N:96:ASP:HB3	4:N:99:LEU:HD22	1.99	0.44
3:R:306:ILE:CD1	3:R:330:LEU:HD13	2.47	0.44
3:W:224:LYS:HE2	3:W:224:LYS:HB3	1.74	0.44
3:2:114:TYR:CD2	3:2:255:ASN:HA	2.52	0.44
3:C:324:VAL:HG23	3:C:326:VAL:H	1.82	0.44
1:F:11:LYS:HE3	4:I:126:TYR:CE1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:128:ASN:HD22	3:M:130:GLU:HB2	1.82	0.44
3:R:128:ASN:HD22	3:R:130:GLU:HB2	1.81	0.44
2:1:109:VAL:O	2:1:113:VAL:HG23	2.18	0.44
2:B:101:GLU:OE1	2:B:101:GLU:HA	2.18	0.44
3:C:107:VAL:HG11	3:H:95:PRO:HG3	2.00	0.44
3:H:162:HIS:HB2	3:H:294:TYR:O	2.16	0.44
1:P:99:LYS:HA	1:P:99:LYS:HD3	1.38	0.44
3:W:374:ASP:OD1	3:W:374:ASP:N	2.35	0.44
5:Y:39:LEU:HD23	5:Y:40:LYS:H	1.83	0.44
2:1:48:LEU:HD23	2:1:48:LEU:HA	1.85	0.44
3:C:186:THR:HG21	3:C:354:ALA:CB	2.46	0.44
4:D:176:SER:HA	4:D:177:PRO:HD3	1.81	0.44
5:E:170:ALA:O	5:E:174:VAL:HG13	2.17	0.44
1:F:127:LYS:O	1:F:130:ALA:HB3	2.17	0.44
3:H:175:MET:HB2	3:H:219:LEU:HD13	1.98	0.44
3:H:277:VAL:O	3:H:294:TYR:HA	2.18	0.44
3:H:334:THR:HA	3:H:386:VAL:HA	2.00	0.44
1:K:101:LEU:HG	1:K:105:LEU:HD12	1.98	0.44
2:L:11:VAL:HA	2:L:130:TYR:HE2	1.82	0.44
3:M:186:THR:HG21	3:M:354:ALA:N	2.33	0.44
1:U:65:ALA:HB2	7:U:201:HEM:HMA1	1.98	0.44
3:W:314:VAL:HA	3:W:315:PRO:HD3	1.77	0.44
3:2:175:MET:HB2	3:2:219:LEU:HD13	1.99	0.44
5:E:38:GLY:O	5:E:39:LEU:HB2	2.18	0.44
2:G:20:VAL:HA	2:G:68:LEU:HD21	2.00	0.44
3:M:345:ASP:OD1	3:M:346:THR:HG22	2.17	0.44
4:N:131:ILE:HG21	4:N:148:LEU:HD22	1.99	0.44
2:1:31:LEU:HD13	2:1:106:LEU:HB2	1.99	0.44
2:G:8:LYS:O	2:G:12:THR:OG1	2.31	0.44
2:Q:31:LEU:HD13	2:Q:106:LEU:HB2	1.99	0.44
3:R:175:MET:HB2	3:R:219:LEU:HD13	1.99	0.44
1:U:106:LEU:HD23	1:U:106:LEU:HA	1.85	0.44
3:W:174:LYS:HB2	3:W:280:TRP:CG	2.52	0.44
3:W:184:GLY:O	3:W:352:GLY:HA3	2.18	0.44
3:W:388:VAL:O	3:W:391:ILE:HG13	2.18	0.44
3:2:336:CYS:SG	3:2:384:VAL:HG23	2.58	0.44
5:4:43:ASP:O	5:4:46:GLU:HG2	2.18	0.44
2:B:11:VAL:HA	2:B:130:TYR:HE2	1.82	0.44
3:C:345:ASP:OD1	3:C:346:THR:HG22	2.18	0.44
2:Q:20:VAL:HA	2:Q:68:LEU:HD21	2.00	0.44
3:2:373:PHE:CZ	3:2:375:LYS:HB2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:312:SER:HB2	3:C:314:VAL:O	2.18	0.44
2:G:51:PRO:O	2:G:55:MET:HG2	2.18	0.44
2:G:101:GLU:OE1	2:G:101:GLU:HA	2.18	0.44
3:H:184:GLY:O	3:H:352:GLY:HA3	2.16	0.44
3:H:206:GLU:H	3:H:206:GLU:HG3	1.62	0.44
5:J:51:LEU:HD23	5:J:51:LEU:HA	1.73	0.44
5:J:122:ILE:HD12	5:J:129:ARG:HH12	1.83	0.44
2:L:31:LEU:HD13	2:L:106:LEU:HB2	2.00	0.44
9:M:1001:NAG:O7	9:M:1001:NAG:O3	2.34	0.44
2:V:92:HIS:HA	2:V:96:LEU:HB2	1.99	0.44
3:W:340:SER:HB3	3:W:344:GLU:N	2.33	0.44
1:Z:85:ASP:N	1:Z:85:ASP:OD1	2.51	0.44
2:1:18:VAL:HG13	2:1:23:VAL:HG21	1.99	0.44
3:C:143:PRO:HG2	3:H:98:ILE:HD13	2.00	0.44
3:C:306:ILE:CD1	3:C:330:LEU:HD13	2.48	0.44
4:N:99:LEU:HD23	4:N:172:LEU:HD23	2.00	0.44
3:R:376:SER:HB2	3:R:380:ALA:O	2.18	0.44
5:T:170:ALA:O	5:T:174:VAL:HG13	2.18	0.44
2:Q:18:VAL:HG13	2:Q:23:VAL:HG21	1.99	0.43
2:Q:101:GLU:HA	2:Q:101:GLU:OE1	2.17	0.43
3:R:118:ARG:O	3:R:119:THR:HB	2.18	0.43
1:U:131:SER:HA	3:W:379:VAL:CG1	2.48	0.43
3:W:391:ILE:O	3:W:395:VAL:HG22	2.18	0.43
3:2:170:PRO:HB2	3:2:259:MET:HG2	2.00	0.43
3:2:174:LYS:HB2	3:2:280:TRP:CG	2.53	0.43
3:2:391:ILE:O	3:2:395:VAL:HG22	2.18	0.43
3:C:160:GLY:HA3	3:C:344:GLU:HG2	2.00	0.43
3:C:334:THR:HA	3:C:386:VAL:HA	2.00	0.43
4:I:145:GLU:OE2	4:I:171:ARG:NH2	2.42	0.43
5:J:61:THR:O	5:J:65:ILE:HG13	2.19	0.43
5:J:175:TRP:HA	5:J:178:LEU:HB2	2.00	0.43
5:O:173:ASP:OD2	5:O:229:LYS:NZ	2.51	0.43
3:W:172:GLN:HE21	3:W:173:ALA:N	2.16	0.43
3:2:128:ASN:HD22	3:2:130:GLU:HB2	1.82	0.43
3:2:186:THR:HG21	3:2:354:ALA:CB	2.48	0.43
3:2:245:LEU:HD11	3:2:395:VAL:HG12	2.00	0.43
3:H:191:GLN:HB3	3:H:192:TRP:CD1	2.53	0.43
3:H:337:ALA:HB3	3:H:385:TYR:HE1	1.83	0.43
3:H:340:SER:OG	3:H:341:LYS:N	2.51	0.43
2:L:45:PHE:HZ	2:L:63:HIS:ND1	2.17	0.43
3:M:296:MET:CE	5:O:71:ARG:HA	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:83:LEU:HD22	1:U:87:HIS:CE1	2.36	0.43
5:Y:122:ILE:HD12	5:Y:129:ARG:HH12	1.83	0.43
3:H:196:THR:HG21	3:H:351:ALA:HB1	2.00	0.43
3:R:312:SER:HB2	3:R:314:VAL:O	2.17	0.43
5:T:44:GLU:OE2	5:T:221:GLY:HA3	2.18	0.43
5:T:122:ILE:HD12	5:T:129:ARG:HH12	1.83	0.43
1:U:127:LYS:O	1:U:130:ALA:HB3	2.19	0.43
2:V:31:LEU:HD13	2:V:106:LEU:HB2	2.00	0.43
5:4:122:ILE:HD12	5:4:129:ARG:HH12	1.83	0.43
1:A:99:LYS:HA	1:A:99:LYS:HD3	1.38	0.43
3:H:183:THR:HB	3:H:199:ASN:ND2	2.20	0.43
2:Q:57:ASN:HB3	2:Q:60:VAL:HG23	2.01	0.43
2:Q:69:GLY:O	2:Q:72:SER:N	2.52	0.43
2:1:92:HIS:HA	2:1:96:LEU:HB2	2.00	0.43
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.85	0.43
1:A:119:PRO:HG2	2:B:55:MET:HG3	2.00	0.43
1:F:27:GLU:OE2	1:F:108:THR:HG23	2.19	0.43
3:M:257:ARG:HG3	3:M:258:VAL:HG23	2.01	0.43
5:O:170:ALA:O	5:O:174:VAL:HG13	2.19	0.43
3:R:181:LEU:HD23	3:R:181:LEU:HA	1.77	0.43
2:V:118:PHE:O	2:V:121:GLU:HB3	2.19	0.43
3:W:135:ASN:O	3:W:139:GLY:N	2.46	0.43
3:W:245:LEU:HD23	3:W:245:LEU:HA	1.63	0.43
3:W:296:MET:CE	5:Y:71:ARG:HA	2.49	0.43
1:Z:35:SER:HB3	2:1:131:GLN:HG3	2.01	0.43
3:2:206:GLU:H	3:2:206:GLU:HG3	1.62	0.43
3:2:267:ASP:CB	3:2:389:THR:HG21	2.48	0.43
3:C:340:SER:OG	3:C:341:LYS:N	2.52	0.43
2:L:69:GLY:O	2:L:72:SER:N	2.51	0.43
3:M:114:TYR:O	3:M:148:VAL:HG23	2.19	0.43
3:M:312:SER:OG	3:M:313:THR:N	2.51	0.43
2:Q:8:LYS:O	2:Q:12:THR:OG1	2.31	0.43
5:Y:46:GLU:HA	5:Y:49:CYS:HB3	1.99	0.43
5:Y:206:SER:HA	9:Y:1002:NAG:H62	1.99	0.43
2:1:41:PHE:HB3	7:1:201:HEM:HMD2	2.00	0.43
5:4:170:ALA:O	5:4:174:VAL:HG13	2.18	0.43
1:A:9:ASN:ND2	1:A:121:VAL:HG22	2.29	0.43
3:C:188:ILE:CG1	3:C:263:LEU:HD11	2.48	0.43
3:C:391:ILE:O	3:C:395:VAL:HG22	2.19	0.43
5:E:166:LYS:HD2	5:E:232:ASP:HB2	2.01	0.43
2:G:18:VAL:HG13	2:G:23:VAL:HG21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:71:PHE:CE2	2:G:137:VAL:HG11	2.53	0.43
2:G:142:ALA:O	2:G:145:TYR:HB2	2.18	0.43
5:J:55:LEU:O	5:J:58:VAL:HG13	2.18	0.43
3:R:162:HIS:HB2	3:R:294:TYR:O	2.18	0.43
3:R:184:GLY:O	3:R:352:GLY:HA3	2.18	0.43
5:T:58:VAL:HG23	5:T:62:LEU:HD12	1.99	0.43
1:U:14:TRP:HE1	1:U:67:THR:HG23	1.83	0.43
5:4:210:LEU:O	5:4:214:ILE:HG12	2.19	0.43
2:B:26:GLU:HG3	2:B:55:MET:HE1	2.00	0.43
3:W:350:ASP:C	3:W:371:LEU:HD12	2.39	0.43
1:Z:131:SER:HA	3:2:379:VAL:CG1	2.49	0.43
3:2:172:GLN:HE21	3:2:173:ALA:N	2.17	0.43
5:4:46:GLU:HA	5:4:49:CYS:HB3	2.01	0.43
3:H:186:THR:HG21	3:H:354:ALA:CB	2.49	0.43
1:K:99:LYS:HA	1:K:99:LYS:HD3	1.40	0.43
3:R:114:TYR:O	3:R:148:VAL:HG23	2.19	0.43
3:R:310:GLU:HA	3:R:319:THR:O	2.19	0.43
5:T:51:LEU:HD23	5:T:51:LEU:HA	1.74	0.43
5:T:166:LYS:HD2	5:T:232:ASP:HB2	2.00	0.43
3:W:306:ILE:CD1	3:W:330:LEU:HD13	2.49	0.43
5:Y:175:TRP:HA	5:Y:178:LEU:HB2	2.01	0.43
5:Y:252:GLY:O	5:Y:256:LYS:HG2	2.19	0.43
5:Y:283:GLU:HG3	5:Y:284:GLU:H	1.83	0.43
2:1:118:PHE:O	2:1:121:GLU:HB3	2.18	0.43
2:B:42:PHE:CE2	7:B:201:HEM:HBC2	2.54	0.42
5:E:210:LEU:O	5:E:214:ILE:HG12	2.19	0.42
1:F:14:TRP:HE1	1:F:67:THR:HG23	1.83	0.42
3:H:128:ASN:HD22	3:H:130:GLU:HB2	1.83	0.42
2:L:44:SER:O	5:O:161:SER:OG	2.22	0.42
3:M:118:ARG:O	3:M:119:THR:HB	2.19	0.42
3:R:191:GLN:HB3	3:R:192:TRP:CD1	2.54	0.42
3:R:257:ARG:HG3	3:R:258:VAL:HG23	2.01	0.42
3:R:334:THR:HA	3:R:386:VAL:HA	2.01	0.42
3:R:337:ALA:HB3	3:R:385:TYR:HE1	1.84	0.42
1:Z:127:LYS:O	1:Z:130:ALA:HB3	2.19	0.42
2:B:31:LEU:HD13	2:B:106:LEU:HB2	2.01	0.42
3:C:206:GLU:H	3:C:206:GLU:HG3	1.59	0.42
5:O:250:THR:OG1	5:O:253:ARG:NH1	2.49	0.42
5:O:283:GLU:HG3	5:O:284:GLU:H	1.84	0.42
4:S:195:GLU:OE1	4:S:216:LYS:HE2	2.19	0.42
5:T:175:TRP:HA	5:T:178:LEU:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:8:LYS:O	2:V:12:THR:OG1	2.31	0.42
2:1:51:PRO:O	2:1:55:MET:HG2	2.19	0.42
3:C:309:TYR:CD1	3:C:328:PRO:HG3	2.53	0.42
2:G:63:HIS:O	2:G:67:VAL:HG23	2.19	0.42
2:G:118:PHE:O	2:G:121:GLU:HB3	2.19	0.42
2:Q:118:PHE:O	2:Q:121:GLU:HB3	2.19	0.42
3:R:174:LYS:HB2	3:R:280:TRP:CG	2.54	0.42
2:V:70:ALA:HB2	7:V:201:HEM:HMA2	2.01	0.42
5:Y:250:THR:OG1	5:Y:253:ARG:NH1	2.51	0.42
2:B:44:SER:O	5:E:161:SER:OG	2.20	0.42
3:C:312:SER:OG	3:C:313:THR:N	2.52	0.42
3:H:391:ILE:O	3:H:395:VAL:HG22	2.19	0.42
5:J:58:VAL:HG23	5:J:62:LEU:HD12	2.00	0.42
3:M:340:SER:OG	3:M:341:LYS:N	2.53	0.42
3:R:186:THR:HG21	3:R:354:ALA:CB	2.49	0.42
3:W:181:LEU:HD23	3:W:181:LEU:HA	1.79	0.42
3:2:118:ARG:O	3:2:119:THR:HB	2.20	0.42
1:F:9:ASN:ND2	1:F:121:VAL:HG22	2.26	0.42
3:H:277:VAL:HG12	3:H:278:SER:O	2.20	0.42
3:R:119:THR:HG23	3:R:121:GLY:CA	2.50	0.42
3:R:277:VAL:O	3:R:294:TYR:HA	2.20	0.42
5:T:283:GLU:HG3	5:T:284:GLU:H	1.84	0.42
1:U:11:LYS:HE3	4:X:126:TYR:CE1	2.55	0.42
1:U:66:LEU:O	1:U:70:VAL:HG12	2.20	0.42
1:U:125:LEU:HD23	1:U:125:LEU:HA	1.85	0.42
3:2:160:GLY:HA3	3:2:344:GLU:HB3	2.00	0.42
5:E:58:VAL:HG23	5:E:62:LEU:HD12	1.99	0.42
3:H:267:ASP:CB	3:H:389:THR:HG21	2.49	0.42
5:J:283:GLU:HG3	5:J:284:GLU:H	1.84	0.42
5:T:210:LEU:O	5:T:214:ILE:HG12	2.20	0.42
3:W:196:THR:HG21	3:W:351:ALA:HB1	2.02	0.42
2:1:11:VAL:HA	2:1:130:TYR:HE2	1.84	0.42
3:2:340:SER:OG	3:2:341:LYS:N	2.52	0.42
2:B:63:HIS:O	2:B:67:VAL:HG23	2.19	0.42
5:E:39:LEU:CD2	5:E:40:LYS:H	2.33	0.42
5:E:122:ILE:HD12	5:E:129:ARG:HH12	1.85	0.42
2:L:92:HIS:O	2:L:97:HIS:N	2.52	0.42
3:M:225:GLN:OE1	3:M:258:VAL:HG21	2.19	0.42
3:W:334:THR:HA	3:W:386:VAL:HA	2.02	0.42
5:Y:44:GLU:OE2	5:Y:221:GLY:HA3	2.20	0.42
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:1002:NAG:O7	9:E:1002:NAG:C3	2.67	0.42
7:G:201:HEM:HHD	7:G:201:HEM:CBC	2.49	0.42
3:H:160:GLY:HA3	3:H:344:GLU:HG2	1.99	0.42
3:M:151:LYS:H	3:M:259:MET:HE1	1.83	0.42
2:1:124:PRO:HB2	2:1:125:PRO:HD3	2.02	0.42
1:A:38:THR:O	1:A:41:THR:HG23	2.20	0.42
3:C:200:LEU:HD12	3:C:217:LEU:HD11	2.02	0.42
2:L:98:VAL:O	2:L:145:TYR:OH	2.22	0.42
1:P:27:GLU:OE2	1:P:108:THR:HG23	2.20	0.42
1:P:127:LYS:O	1:P:130:ALA:HB3	2.19	0.42
2:Q:92:HIS:HA	2:Q:96:LEU:HB2	2.01	0.42
3:W:340:SER:OG	3:W:341:LYS:N	2.53	0.42
1:Z:14:TRP:HE1	1:Z:67:THR:HG23	1.85	0.42
1:Z:83:LEU:HD22	1:Z:87:HIS:CE1	2.35	0.42
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.73	0.42
3:C:118:ARG:O	3:C:119:THR:HB	2.20	0.42
3:H:147:ALA:HB1	3:H:254:VAL:HG21	2.02	0.42
2:L:11:VAL:HG13	2:L:130:TYR:CZ	2.55	0.42
5:T:61:THR:O	5:T:65:ILE:HG13	2.20	0.42
3:2:188:ILE:CG1	3:2:263:LEU:HD11	2.50	0.42
2:B:41:PHE:HB3	7:B:201:HEM:HMD2	2.01	0.41
3:C:198:LYS:HZ1	3:C:329:ILE:HD11	1.84	0.41
5:E:283:GLU:HG3	5:E:284:GLU:H	1.85	0.41
2:G:124:PRO:HB2	2:G:125:PRO:HD3	2.02	0.41
3:H:376:SER:HB2	3:H:380:ALA:O	2.20	0.41
5:J:206:SER:HA	9:J:1002:NAG:O6	2.19	0.41
2:L:20:VAL:HA	2:L:68:LEU:HD21	2.01	0.41
3:M:147:ALA:HB1	3:M:254:VAL:HG21	2.02	0.41
3:R:183:THR:HB	3:R:199:ASN:ND2	2.20	0.41
3:R:267:ASP:CB	3:R:389:THR:HG21	2.50	0.41
3:W:114:TYR:O	3:W:148:VAL:HG23	2.20	0.41
1:Z:99:LYS:HA	1:Z:99:LYS:HD3	1.41	0.41
5:4:283:GLU:HG3	5:4:284:GLU:H	1.85	0.41
1:A:101:LEU:HG	1:A:105:LEU:HD12	2.01	0.41
5:J:41:THR:OG1	5:J:42:LYS:N	2.53	0.41
2:L:102:ASN:HA	2:L:105:LEU:HB2	2.01	0.41
2:L:124:PRO:HB2	2:L:125:PRO:HD3	2.02	0.41
3:R:119:THR:C	3:R:121:GLY:HA3	2.40	0.41
3:R:198:LYS:NZ	3:R:329:ILE:HD11	2.35	0.41
1:U:109:LEU:HA	1:U:109:LEU:HD23	1.82	0.41
5:Y:210:LEU:O	5:Y:214:ILE:HG12	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:350:ASP:C	3:2:371:LEU:HD12	2.41	0.41
3:2:388:VAL:O	3:2:391:ILE:HG13	2.20	0.41
1:K:32:MET:SD	1:K:101:LEU:HB2	2.60	0.41
7:Q:201:HEM:HBB2	7:Q:201:HEM:CHC	2.39	0.41
3:R:188:ILE:CG1	3:R:263:LEU:HD11	2.50	0.41
5:T:126:THR:HG23	5:T:127:SER:H	1.85	0.41
1:U:46:PHE:HZ	7:U:201:HEM:O1D	2.03	0.41
2:V:71:PHE:CE2	2:V:137:VAL:HG11	2.55	0.41
5:4:97:LEU:O	5:4:100:VAL:HG12	2.20	0.41
3:C:225:GLN:OE1	3:C:258:VAL:HG21	2.19	0.41
4:D:99:LEU:HD23	4:D:172:LEU:HD23	2.02	0.41
5:E:55:LEU:O	5:E:58:VAL:HG13	2.20	0.41
3:H:212:ASP:OD1	3:H:212:ASP:N	2.53	0.41
5:O:97:LEU:O	5:O:100:VAL:HG12	2.20	0.41
4:X:145:GLU:OE2	4:X:171:ARG:NH2	2.42	0.41
1:Z:9:ASN:ND2	1:Z:121:VAL:HG22	2.26	0.41
3:2:163:LEU:HD22	3:2:164:ASP:H	1.85	0.41
5:4:55:LEU:O	5:4:58:VAL:HG13	2.20	0.41
3:C:174:LYS:HB2	3:C:280:TRP:CG	2.55	0.41
3:C:345:ASP:CG	3:C:346:THR:N	2.69	0.41
1:F:83:LEU:HD22	1:F:87:HIS:CE1	2.36	0.41
1:K:3:SER:N	1:K:6:ASP:OD2	2.44	0.41
3:M:110:GLN:N	3:R:102:TYR:O	2.40	0.41
3:M:200:LEU:HD12	3:M:217:LEU:HD11	2.02	0.41
3:R:113:ASN:N	3:R:113:ASN:OD1	2.53	0.41
3:R:345:ASP:CG	3:R:346:THR:N	2.70	0.41
4:S:90:LEU:HD22	4:S:156:TRP:HB2	2.02	0.41
1:U:87:HIS:NE2	7:U:201:HEM:NA	2.68	0.41
2:V:41:PHE:HB3	7:V:201:HEM:HMD2	2.02	0.41
2:1:92:HIS:O	2:1:97:HIS:N	2.53	0.41
3:C:279:GLY:O	3:C:292:LEU:HD12	2.20	0.41
5:E:250:THR:OG1	5:E:253:ARG:NH1	2.50	0.41
2:G:92:HIS:O	2:G:97:HIS:N	2.53	0.41
3:H:174:LYS:HB2	3:H:280:TRP:CG	2.56	0.41
3:H:181:LEU:HD23	3:H:181:LEU:HA	1.78	0.41
3:H:225:GLN:OE1	3:H:258:VAL:HG21	2.20	0.41
2:L:63:HIS:O	2:L:67:VAL:HG23	2.20	0.41
3:M:395:VAL:O	3:M:399:ILE:HG12	2.20	0.41
5:O:39:LEU:CD2	5:O:40:LYS:H	2.34	0.41
5:O:44:GLU:OE2	5:O:221:GLY:HA3	2.21	0.41
2:Q:98:VAL:O	2:Q:145:TYR:OH	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:83:LEU:HD23	1:U:83:LEU:HA	1.95	0.41
2:V:98:VAL:O	2:V:145:TYR:OH	2.26	0.41
3:W:160:GLY:HA3	3:W:344:GLU:HG2	2.03	0.41
3:W:373:PHE:CZ	3:W:375:LYS:HB2	2.56	0.41
5:Y:39:LEU:CD2	5:Y:40:LYS:H	2.34	0.41
1:Z:107:VAL:HG11	2:1:127:GLN:OE1	2.19	0.41
3:2:334:THR:HA	3:2:386:VAL:HA	2.03	0.41
7:A:201:HEM:HMB1	7:A:201:HEM:HBB2	2.03	0.41
2:B:118:PHE:O	2:B:121:GLU:HB3	2.21	0.41
9:J:1002:NAG:O7	9:J:1002:NAG:O3	2.37	0.41
5:O:42:LYS:O	5:O:42:LYS:HG2	2.20	0.41
3:R:147:ALA:HB1	3:R:254:VAL:HG21	2.03	0.41
2:V:11:VAL:HA	2:V:130:TYR:HE2	1.86	0.41
2:V:105:LEU:HD23	2:V:105:LEU:HA	1.92	0.41
3:W:395:VAL:O	3:W:399:ILE:HG12	2.20	0.41
5:Y:226:HIS:HB3	5:Y:229:LYS:HE2	2.02	0.41
2:1:142:ALA:O	2:1:145:TYR:HB2	2.20	0.41
5:4:76:VAL:HG13	5:4:146:ARG:HG3	2.03	0.41
5:E:44:GLU:OE2	5:E:221:GLY:HA3	2.21	0.41
5:J:39:LEU:H	5:J:223:LEU:HD21	1.84	0.41
1:K:11:LYS:HE3	4:N:126:TYR:CE1	2.56	0.41
5:O:46:GLU:HA	5:O:49:CYS:HB3	2.02	0.41
5:O:122:ILE:HD12	5:O:129:ARG:HH12	1.86	0.41
4:S:140:THR:OG1	4:S:143:LYS:O	2.35	0.41
5:T:126:THR:HG23	5:T:127:SER:N	2.36	0.41
7:U:201:HEM:HMB2	7:U:201:HEM:HBB2	2.01	0.41
5:Y:126:THR:HG23	5:Y:127:SER:H	1.85	0.41
3:2:345:ASP:OD1	3:2:346:THR:HG22	2.21	0.41
3:C:395:VAL:O	3:C:399:ILE:HG12	2.20	0.41
5:E:56:LYS:HE2	5:E:56:LYS:HA	2.03	0.41
5:J:56:LYS:HE2	5:J:56:LYS:HA	2.03	0.41
1:K:14:TRP:HE1	1:K:67:THR:HG23	1.86	0.41
1:K:48:LEU:HD23	1:K:48:LEU:HA	1.75	0.41
1:K:119:PRO:HG2	2:L:55:MET:HG3	2.02	0.41
1:K:125:LEU:HD23	1:K:125:LEU:HA	1.87	0.41
3:M:273:ARG:HH11	3:M:273:ARG:HG2	1.85	0.41
3:M:309:TYR:CD1	3:M:328:PRO:HG3	2.55	0.41
9:O:1002:NAG:O7	9:O:1002:NAG:O3	2.32	0.41
2:Q:124:PRO:HB2	2:Q:125:PRO:HD3	2.03	0.41
3:R:212:ASP:OD1	3:R:212:ASP:N	2.54	0.41
3:W:206:GLU:H	3:W:206:GLU:HG3	1.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:99:LEU:HD23	4:X:172:LEU:HD23	2.03	0.41
5:Y:126:THR:HG23	5:Y:127:SER:N	2.36	0.41
3:2:306:ILE:CD1	3:2:330:LEU:HD13	2.49	0.41
4:3:140:THR:OG1	4:3:143:LYS:O	2.35	0.41
5:4:58:VAL:HG23	5:4:62:LEU:HD12	2.02	0.41
1:A:127:LYS:O	1:A:130:ALA:HB3	2.21	0.41
3:C:151:LYS:H	3:C:259:MET:HE1	1.84	0.41
5:E:226:HIS:HB3	5:E:229:LYS:HE2	2.03	0.41
3:H:119:THR:HG23	3:H:121:GLY:CA	2.48	0.41
3:H:194:LEU:HD13	3:H:370:ILE:HG13	2.03	0.41
3:H:257:ARG:HG3	3:H:258:VAL:HG23	2.03	0.41
2:L:8:LYS:O	2:L:12:THR:OG1	2.30	0.41
3:M:206:GLU:H	3:M:206:GLU:HG3	1.61	0.41
2:Q:51:PRO:O	2:Q:55:MET:HG2	2.21	0.41
2:V:20:VAL:HA	2:V:68:LEU:HD21	2.02	0.41
3:W:191:GLN:HB3	3:W:192:TRP:CD1	2.56	0.41
3:W:269:ALA:O	3:W:299:VAL:HG21	2.21	0.41
5:Y:173:ASP:OD2	5:Y:229:LYS:NZ	2.54	0.41
5:4:61:THR:O	5:4:65:ILE:HG13	2.21	0.41
2:B:48:LEU:CD2	2:B:54:VAL:HG22	2.51	0.40
3:C:175:MET:HB2	3:C:219:LEU:HD13	2.01	0.40
5:J:97:LEU:O	5:J:100:VAL:HG12	2.21	0.40
5:J:126:THR:HG23	5:J:127:SER:H	1.86	0.40
5:O:70:GLU:O	5:O:74:VAL:HG13	2.21	0.40
1:P:11:LYS:NZ	4:S:151:ASN:OD1	2.49	0.40
2:Q:26:GLU:HA	2:Q:55:MET:HE1	2.03	0.40
5:Y:40:LYS:HG2	5:Y:41:THR:H	1.85	0.40
3:2:314:VAL:HA	3:2:315:PRO:HD3	1.78	0.40
5:4:126:THR:HG23	5:4:127:SER:N	2.37	0.40
5:E:40:LYS:HG2	5:E:41:THR:H	1.86	0.40
1:F:106:LEU:HD23	1:F:106:LEU:HA	1.85	0.40
2:G:92:HIS:HA	2:G:96:LEU:HB2	2.02	0.40
3:H:312:SER:OG	3:H:313:THR:N	2.54	0.40
5:J:68:THR:HG22	5:J:69:THR:HG23	2.02	0.40
3:W:200:LEU:HD12	3:W:217:LEU:HD11	2.04	0.40
5:Y:256:LYS:HE3	5:Y:256:LYS:HB3	1.80	0.40
1:Z:38:THR:O	1:Z:41:THR:HG23	2.20	0.40
7:1:201:HEM:HHD	7:1:201:HEM:CBC	2.50	0.40
3:2:114:TYR:O	3:2:148:VAL:HG23	2.21	0.40
3:2:179:HIS:CE1	3:2:203:ASN:HB2	2.56	0.40
3:2:277:VAL:O	3:2:294:TYR:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:44:GLU:OE2	5:4:221:GLY:HA3	2.21	0.40
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.96	0.40
3:C:150:GLY:HA2	3:C:365:TRP:HB2	2.03	0.40
3:H:198:LYS:NZ	3:H:329:ILE:HD11	2.36	0.40
1:P:35:SER:HB3	2:Q:131:GLN:HG3	2.04	0.40
1:P:85:ASP:N	1:P:85:ASP:OD1	2.54	0.40
2:Q:48:LEU:CD2	2:Q:54:VAL:HG22	2.51	0.40
3:R:277:VAL:HG12	3:R:278:SER:O	2.21	0.40
2:V:25:GLY:HA3	2:V:61:LYS:HA	2.03	0.40
3:W:340:SER:HB3	3:W:344:GLU:H	1.84	0.40
2:1:20:VAL:HA	2:1:68:LEU:HD21	2.04	0.40
5:4:39:LEU:H	5:4:223:LEU:HD21	1.85	0.40
1:A:11:LYS:HE3	4:D:126:TYR:CE1	2.56	0.40
1:A:35:SER:HB3	2:B:131:GLN:HG3	2.03	0.40
2:B:92:HIS:O	2:B:97:HIS:N	2.54	0.40
3:C:191:GLN:HB3	3:C:192:TRP:CD1	2.57	0.40
5:E:42:LYS:O	5:E:42:LYS:HG2	2.21	0.40
5:J:126:THR:HG23	5:J:127:SER:N	2.37	0.40
1:K:38:THR:O	1:K:41:THR:HG23	2.21	0.40
3:R:395:VAL:O	3:R:399:ILE:HG12	2.21	0.40
5:T:80:LYS:HB2	5:T:146:ARG:NE	2.36	0.40
2:V:104:ARG:HE	2:V:104:ARG:HB3	1.68	0.40
5:Y:170:ALA:O	5:Y:174:VAL:HG13	2.21	0.40
3:2:273:ARG:HH11	3:2:273:ARG:HG2	1.86	0.40
5:4:175:TRP:HA	5:4:178:LEU:HB2	2.03	0.40
5:4:256:LYS:HE3	5:4:260:LYS:HE3	2.03	0.40
2:B:11:VAL:HG13	2:B:130:TYR:CZ	2.57	0.40
1:K:131:SER:HA	3:M:379:VAL:CG1	2.52	0.40
3:M:371:LEU:HA	3:M:385:TYR:CD2	2.57	0.40
5:O:40:LYS:HG2	5:O:41:THR:H	1.86	0.40
5:T:55:LEU:O	5:T:58:VAL:HG13	2.21	0.40
5:T:226:HIS:HB3	5:T:229:LYS:HE2	2.04	0.40
1:U:85:ASP:N	1:U:85:ASP:OD1	2.54	0.40
2:V:24:GLY:N	2:V:68:LEU:HD22	2.26	0.40
3:W:119:THR:HG23	3:W:121:GLY:CA	2.51	0.40
3:W:273:ARG:HH11	3:W:273:ARG:HG2	1.86	0.40
5:Y:283:GLU:HG3	5:Y:284:GLU:N	2.37	0.40
3:2:92:CYS:O	3:2:92:CYS:SG	2.79	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%)	130 (94%)	9 (6%)	0	100	100
1	F	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
1	K	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
1	P	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
1	U	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
1	Z	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
2	1	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	B	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	G	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
2	L	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	Q	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	V	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
3	2	306/315 (97%)	283 (92%)	23 (8%)	0	100	100
3	C	306/315 (97%)	285 (93%)	21 (7%)	0	100	100
3	H	306/315 (97%)	283 (92%)	23 (8%)	0	100	100
3	M	306/315 (97%)	282 (92%)	24 (8%)	0	100	100
3	R	306/315 (97%)	283 (92%)	23 (8%)	0	100	100
3	W	306/315 (97%)	283 (92%)	23 (8%)	0	100	100
4	3	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
4	D	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
4	I	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
4	N	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
4	S	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
4	X	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
5	4	259/343 (76%)	232 (90%)	26 (10%)	1 (0%)	34	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	259/343 (76%)	231 (89%)	27 (10%)	1 (0%)	34	69
5	J	259/343 (76%)	234 (90%)	24 (9%)	1 (0%)	34	69
5	O	259/343 (76%)	232 (90%)	26 (10%)	1 (0%)	34	69
5	T	259/343 (76%)	233 (90%)	25 (10%)	1 (0%)	34	69
5	Y	259/343 (76%)	232 (90%)	26 (10%)	1 (0%)	34	69
All	All	5940/6546 (91%)	5522 (93%)	412 (7%)	6 (0%)	51	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	39	LEU
5	J	39	LEU
5	O	39	LEU
5	T	39	LEU
5	Y	39	LEU
5	4	39	LEU

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	113/113 (100%)	100 (88%)	13 (12%)	5	22
1	F	113/113 (100%)	100 (88%)	13 (12%)	5	22
1	K	113/113 (100%)	100 (88%)	13 (12%)	5	22
1	P	113/113 (100%)	100 (88%)	13 (12%)	5	22
1	U	113/113 (100%)	101 (89%)	12 (11%)	6	26
1	Z	113/113 (100%)	100 (88%)	13 (12%)	5	22
2	1	118/118 (100%)	106 (90%)	12 (10%)	7	27
2	B	118/118 (100%)	107 (91%)	11 (9%)	9	32
2	G	118/118 (100%)	107 (91%)	11 (9%)	9	32
2	L	118/118 (100%)	106 (90%)	12 (10%)	7	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	118/118 (100%)	108 (92%)	10 (8%)	10	37
2	V	118/118 (100%)	106 (90%)	12 (10%)	7	27
3	2	266/271 (98%)	238 (90%)	28 (10%)	7	26
3	C	266/271 (98%)	237 (89%)	29 (11%)	6	25
3	H	266/271 (98%)	237 (89%)	29 (11%)	6	25
3	M	266/271 (98%)	235 (88%)	31 (12%)	5	22
3	R	266/271 (98%)	235 (88%)	31 (12%)	5	22
3	W	266/271 (98%)	236 (89%)	30 (11%)	6	23
4	3	133/134 (99%)	129 (97%)	4 (3%)	41	71
4	D	133/134 (99%)	129 (97%)	4 (3%)	41	71
4	I	133/134 (99%)	127 (96%)	6 (4%)	27	60
4	N	133/134 (99%)	129 (97%)	4 (3%)	41	71
4	S	133/134 (99%)	128 (96%)	5 (4%)	33	66
4	X	133/134 (99%)	128 (96%)	5 (4%)	33	66
5	4	202/272 (74%)	180 (89%)	22 (11%)	6	25
5	E	202/272 (74%)	178 (88%)	24 (12%)	5	20
5	J	202/272 (74%)	180 (89%)	22 (11%)	6	25
5	O	202/272 (74%)	179 (89%)	23 (11%)	5	23
5	T	202/272 (74%)	180 (89%)	22 (11%)	6	25
5	Y	202/272 (74%)	180 (89%)	22 (11%)	6	25
All	All	4992/5448 (92%)	4506 (90%)	486 (10%)	8	30

All (486) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	23	GLU
1	A	38	THR
1	A	45	HIS
1	A	50	HIS
1	A	67	THR
1	A	70	VAL
1	A	72	HIS
1	A	76	MET
1	A	80	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	92	ARG
1	A	124	SER
1	A	133	SER
2	B	3	LEU
2	B	4	THR
2	B	6	GLU
2	B	12	THR
2	B	22	GLU
2	B	50	THR
2	B	87	THR
2	B	95	LYS
2	B	104	ARG
2	B	145	TYR
2	B	146	HIS
3	C	97	GLU
3	C	120	GLU
3	C	122	ASP
3	C	130	GLU
3	C	148	VAL
3	C	154	ASN
3	C	166	LYS
3	C	176	VAL
3	C	179	HIS
3	C	188	ILE
3	C	191	GLN
3	C	193	LEU
3	C	200	LEU
3	C	221	VAL
3	C	224	LYS
3	C	253	SER
3	C	259	MET
3	C	268	TYR
3	C	278	SER
3	C	297	LEU
3	C	314	VAL
3	C	323	PRO
3	C	326	VAL
3	C	340	SER
3	C	362	GLU
3	C	368	THR
3	C	386	VAL
3	C	388	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	395	VAL
4	D	99	LEU
4	D	171	ARG
4	D	189	VAL
4	D	217	LEU
5	E	37	GLU
5	E	39	LEU
5	E	41	THR
5	E	46	GLU
5	E	51	LEU
5	E	56	LYS
5	E	58	VAL
5	E	68	THR
5	E	76	VAL
5	E	97	LEU
5	E	106	ARG
5	E	107	LEU
5	E	142	VAL
5	E	153	ARG
5	E	174	VAL
5	E	178	LEU
5	E	190	VAL
5	E	205	THR
5	E	206	SER
5	E	210	LEU
5	E	233	VAL
5	E	237	PHE
5	E	243	SER
5	E	282	ILE
1	F	1	VAL
1	F	23	GLU
1	F	38	THR
1	F	45	HIS
1	F	50	HIS
1	F	67	THR
1	F	70	VAL
1	F	72	HIS
1	F	76	MET
1	F	80	LEU
1	F	92	ARG
1	F	124	SER
1	F	133	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	3	LEU
2	G	4	THR
2	G	6	GLU
2	G	12	THR
2	G	31	LEU
2	G	50	THR
2	G	87	THR
2	G	95	LYS
2	G	104	ARG
2	G	145	TYR
2	G	146	HIS
3	H	97	GLU
3	H	120	GLU
3	H	122	ASP
3	H	130	GLU
3	H	148	VAL
3	H	154	ASN
3	H	166	LYS
3	H	176	VAL
3	H	179	HIS
3	H	188	ILE
3	H	191	GLN
3	H	193	LEU
3	H	200	LEU
3	H	221	VAL
3	H	224	LYS
3	H	253	SER
3	H	259	MET
3	H	268	TYR
3	H	278	SER
3	H	297	LEU
3	H	314	VAL
3	H	326	VAL
3	H	340	SER
3	H	347	CYS
3	H	357	VAL
3	H	368	THR
3	H	371	LEU
3	H	386	VAL
3	H	388	VAL
4	I	90	LEU
4	I	99	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	I	113	ASN
4	I	171	ARG
4	I	189	VAL
4	I	217	LEU
5	J	37	GLU
5	J	39	LEU
5	J	41	THR
5	J	51	LEU
5	J	56	LYS
5	J	58	VAL
5	J	68	THR
5	J	76	VAL
5	J	97	LEU
5	J	106	ARG
5	J	142	VAL
5	J	153	ARG
5	J	174	VAL
5	J	178	LEU
5	J	190	VAL
5	J	205	THR
5	J	206	SER
5	J	210	LEU
5	J	233	VAL
5	J	237	PHE
5	J	243	SER
5	J	282	ILE
1	K	1	VAL
1	K	23	GLU
1	K	38	THR
1	K	45	HIS
1	K	50	HIS
1	K	67	THR
1	K	70	VAL
1	K	72	HIS
1	K	76	MET
1	K	80	LEU
1	K	92	ARG
1	K	124	SER
1	K	133	SER
2	L	3	LEU
2	L	4	THR
2	L	6	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	12	THR
2	L	22	GLU
2	L	31	LEU
2	L	50	THR
2	L	87	THR
2	L	95	LYS
2	L	104	ARG
2	L	145	TYR
2	L	146	HIS
3	M	97	GLU
3	M	103	VAL
3	M	120	GLU
3	M	122	ASP
3	M	130	GLU
3	M	148	VAL
3	M	154	ASN
3	M	157	ASN
3	M	166	LYS
3	M	176	VAL
3	M	179	HIS
3	M	191	GLN
3	M	193	LEU
3	M	200	LEU
3	M	221	VAL
3	M	224	LYS
3	M	253	SER
3	M	259	MET
3	M	268	TYR
3	M	278	SER
3	M	297	LEU
3	M	314	VAL
3	M	323	PRO
3	M	326	VAL
3	M	347	CYS
3	M	357	VAL
3	M	362	GLU
3	M	368	THR
3	M	371	LEU
3	M	386	VAL
3	M	388	VAL
4	N	99	LEU
4	N	171	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	N	189	VAL
4	N	217	LEU
5	O	37	GLU
5	O	39	LEU
5	O	41	THR
5	O	51	LEU
5	O	56	LYS
5	O	58	VAL
5	O	68	THR
5	O	76	VAL
5	O	97	LEU
5	O	106	ARG
5	O	107	LEU
5	O	142	VAL
5	O	153	ARG
5	O	174	VAL
5	O	178	LEU
5	O	190	VAL
5	O	205	THR
5	O	206	SER
5	O	210	LEU
5	O	233	VAL
5	O	237	PHE
5	O	243	SER
5	O	282	ILE
1	P	1	VAL
1	P	23	GLU
1	P	38	THR
1	P	45	HIS
1	P	50	HIS
1	P	67	THR
1	P	70	VAL
1	P	72	HIS
1	P	76	MET
1	P	80	LEU
1	P	92	ARG
1	P	124	SER
1	P	133	SER
2	Q	3	LEU
2	Q	4	THR
2	Q	6	GLU
2	Q	12	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Q	50	THR
2	Q	87	THR
2	Q	95	LYS
2	Q	104	ARG
2	Q	145	TYR
2	Q	146	HIS
3	R	97	GLU
3	R	120	GLU
3	R	122	ASP
3	R	130	GLU
3	R	148	VAL
3	R	154	ASN
3	R	157	ASN
3	R	166	LYS
3	R	176	VAL
3	R	179	HIS
3	R	191	GLN
3	R	193	LEU
3	R	200	LEU
3	R	221	VAL
3	R	224	LYS
3	R	253	SER
3	R	259	MET
3	R	268	TYR
3	R	278	SER
3	R	297	LEU
3	R	314	VAL
3	R	326	VAL
3	R	340	SER
3	R	347	CYS
3	R	357	VAL
3	R	362	GLU
3	R	368	THR
3	R	371	LEU
3	R	386	VAL
3	R	388	VAL
3	R	395	VAL
4	S	99	LEU
4	S	117	LEU
4	S	171	ARG
4	S	189	VAL
4	S	217	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	T	37	GLU
5	T	39	LEU
5	T	41	THR
5	T	51	LEU
5	T	56	LYS
5	T	58	VAL
5	T	68	THR
5	T	76	VAL
5	T	97	LEU
5	T	106	ARG
5	T	142	VAL
5	T	153	ARG
5	T	174	VAL
5	T	178	LEU
5	T	190	VAL
5	T	205	THR
5	T	206	SER
5	T	210	LEU
5	T	233	VAL
5	T	237	PHE
5	T	243	SER
5	T	282	ILE
1	U	23	GLU
1	U	38	THR
1	U	45	HIS
1	U	50	HIS
1	U	67	THR
1	U	70	VAL
1	U	72	HIS
1	U	76	MET
1	U	80	LEU
1	U	92	ARG
1	U	124	SER
1	U	133	SER
2	V	3	LEU
2	V	4	THR
2	V	6	GLU
2	V	12	THR
2	V	22	GLU
2	V	31	LEU
2	V	50	THR
2	V	87	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	V	95	LYS
2	V	104	ARG
2	V	145	TYR
2	V	146	HIS
3	W	97	GLU
3	W	120	GLU
3	W	122	ASP
3	W	127	LEU
3	W	130	GLU
3	W	148	VAL
3	W	154	ASN
3	W	166	LYS
3	W	176	VAL
3	W	179	HIS
3	W	188	ILE
3	W	191	GLN
3	W	193	LEU
3	W	200	LEU
3	W	221	VAL
3	W	224	LYS
3	W	253	SER
3	W	259	MET
3	W	268	TYR
3	W	278	SER
3	W	297	LEU
3	W	314	VAL
3	W	326	VAL
3	W	340	SER
3	W	347	CYS
3	W	362	GLU
3	W	368	THR
3	W	371	LEU
3	W	386	VAL
3	W	388	VAL
4	X	99	LEU
4	X	117	LEU
4	X	171	ARG
4	X	189	VAL
4	X	217	LEU
5	Y	37	GLU
5	Y	39	LEU
5	Y	41	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	Y	51	LEU
5	Y	56	LYS
5	Y	58	VAL
5	Y	68	THR
5	Y	76	VAL
5	Y	97	LEU
5	Y	106	ARG
5	Y	142	VAL
5	Y	153	ARG
5	Y	174	VAL
5	Y	178	LEU
5	Y	190	VAL
5	Y	205	THR
5	Y	206	SER
5	Y	210	LEU
5	Y	233	VAL
5	Y	237	PHE
5	Y	243	SER
5	Y	282	ILE
1	Z	1	VAL
1	Z	23	GLU
1	Z	38	THR
1	Z	45	HIS
1	Z	50	HIS
1	Z	67	THR
1	Z	70	VAL
1	Z	72	HIS
1	Z	76	MET
1	Z	80	LEU
1	Z	92	ARG
1	Z	124	SER
1	Z	133	SER
2	1	3	LEU
2	1	4	THR
2	1	6	GLU
2	1	12	THR
2	1	22	GLU
2	1	31	LEU
2	1	50	THR
2	1	87	THR
2	1	95	LYS
2	1	104	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	145	TYR
2	1	146	HIS
3	2	97	GLU
3	2	120	GLU
3	2	122	ASP
3	2	130	GLU
3	2	148	VAL
3	2	154	ASN
3	2	166	LYS
3	2	176	VAL
3	2	179	HIS
3	2	191	GLN
3	2	193	LEU
3	2	200	LEU
3	2	221	VAL
3	2	224	LYS
3	2	253	SER
3	2	259	MET
3	2	268	TYR
3	2	278	SER
3	2	297	LEU
3	2	314	VAL
3	2	326	VAL
3	2	340	SER
3	2	347	CYS
3	2	357	VAL
3	2	368	THR
3	2	371	LEU
3	2	386	VAL
3	2	388	VAL
4	3	99	LEU
4	3	171	ARG
4	3	189	VAL
4	3	217	LEU
5	4	37	GLU
5	4	39	LEU
5	4	41	THR
5	4	51	LEU
5	4	56	LYS
5	4	58	VAL
5	4	68	THR
5	4	76	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	4	97	LEU
5	4	106	ARG
5	4	142	VAL
5	4	153	ARG
5	4	174	VAL
5	4	178	LEU
5	4	190	VAL
5	4	205	THR
5	4	206	SER
5	4	210	LEU
5	4	233	VAL
5	4	237	PHE
5	4	243	SER
5	4	282	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
2	B	131	GLN
3	C	327	GLN
4	D	113	ASN
5	E	54	GLN
1	F	9	ASN
2	G	131	GLN
3	H	100	HIS
3	H	157	ASN
3	H	327	GLN
3	H	358	HIS
5	J	54	GLN
1	K	9	ASN
3	M	157	ASN
3	M	327	GLN
4	N	113	ASN
5	O	54	GLN
1	P	9	ASN
2	Q	131	GLN
3	R	100	HIS
3	R	327	GLN
4	S	113	ASN
5	T	54	GLN
1	U	9	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	W	172	GLN
3	W	327	GLN
4	X	165	ASN
5	Y	54	GLN
1	Z	9	ASN
2	1	131	GLN
3	2	100	HIS
3	2	327	GLN
5	4	54	GLN

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)

20 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	$\#\|Z\| > 2$
6	NAG	a	1	6,3	14,14,15	1.14	1 (7%)	17,19,21	1.74	2 (11%)
6	NAG	a	2	6	14,14,15	1.14	1 (7%)	17,19,21	1.20	1 (5%)
6	NAG	b	1	6,3	14,14,15	0.59	0	17,19,21	2.02	5 (29%)
6	NAG	b	2	6	14,14,15	0.24	0	17,19,21	0.63	0
6	NAG	c	1	6,3	14,14,15	1.01	1 (7%)	17,19,21	1.99	5 (29%)
6	NAG	c	2	6	14,14,15	0.58	0	17,19,21	0.81	1 (5%)
6	NAG	d	1	6,3	14,14,15	0.49	0	17,19,21	2.08	2 (11%)
6	NAG	d	2	6	14,14,15	1.19	2 (14%)	17,19,21	1.13	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	e	1	6,3	14,14,15	0.93	1 (7%)	17,19,21	1.66	5 (29%)
6	NAG	e	2	6	14,14,15	0.33	0	17,19,21	0.77	1 (5%)
6	NAG	f	1	6,3	14,14,15	0.53	0	17,19,21	1.59	2 (11%)
6	NAG	f	2	6	14,14,15	1.28	2 (14%)	17,19,21	1.14	1 (5%)
6	NAG	g	1	6,3	14,14,15	0.83	1 (7%)	17,19,21	1.67	4 (23%)
6	NAG	g	2	6	14,14,15	0.54	0	17,19,21	0.82	1 (5%)
6	NAG	h	1	6,3	14,14,15	0.78	1 (7%)	17,19,21	1.92	5 (29%)
6	NAG	h	2	6	14,14,15	0.34	0	17,19,21	0.77	1 (5%)
6	NAG	i	1	6,3	14,14,15	0.36	0	17,19,21	1.32	1 (5%)
6	NAG	i	2	6	14,14,15	0.78	1 (7%)	17,19,21	0.87	1 (5%)
6	NAG	j	1	6,3	14,14,15	0.83	1 (7%)	17,19,21	1.77	5 (29%)
6	NAG	j	2	6	14,14,15	0.51	0	17,19,21	0.86	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	a	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	1/6/23/26	0/1/1/1
6	NAG	b	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	b	2	6	-	3/6/23/26	0/1/1/1
6	NAG	c	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	c	2	6	-	3/6/23/26	0/1/1/1
6	NAG	d	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	d	2	6	-	2/6/23/26	0/1/1/1
6	NAG	e	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	e	2	6	-	2/6/23/26	0/1/1/1
6	NAG	f	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	NAG	g	1	6,3	-	4/6/23/26	0/1/1/1
6	NAG	g	2	6	-	3/6/23/26	0/1/1/1
6	NAG	h	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	h	2	6	-	4/6/23/26	0/1/1/1
6	NAG	i	1	6,3	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	i	2	6	-	0/6/23/26	0/1/1/1
6	NAG	j	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	j	2	6	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	2	NAG	O5-C1	4.21	1.50	1.43
6	a	1	NAG	O5-C1	3.90	1.50	1.43
6	a	2	NAG	O5-C1	3.72	1.49	1.43
6	d	2	NAG	O5-C1	3.48	1.49	1.43
6	c	1	NAG	O5-C1	3.27	1.48	1.43
6	e	1	NAG	C1-C2	2.87	1.56	1.52
6	j	1	NAG	O5-C1	2.71	1.48	1.43
6	d	2	NAG	C1-C2	2.63	1.56	1.52
6	g	1	NAG	O5-C1	-2.53	1.39	1.43
6	i	2	NAG	C1-C2	2.19	1.55	1.52
6	h	1	NAG	O5-C1	2.17	1.47	1.43
6	f	2	NAG	C1-C2	2.13	1.55	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	d	1	NAG	C1-O5-C5	7.29	122.06	112.19
6	a	1	NAG	C1-O5-C5	5.81	120.06	112.19
6	b	1	NAG	C1-O5-C5	5.15	119.17	112.19
6	f	1	NAG	C1-O5-C5	5.09	119.09	112.19
6	c	1	NAG	C1-O5-C5	4.61	118.43	112.19
6	h	1	NAG	C1-O5-C5	4.57	118.39	112.19
6	g	1	NAG	C1-O5-C5	4.56	118.37	112.19
6	a	2	NAG	C1-O5-C5	4.13	117.78	112.19
6	f	2	NAG	C1-O5-C5	4.06	117.69	112.19
6	j	1	NAG	C1-O5-C5	4.03	117.65	112.19
6	d	2	NAG	C1-O5-C5	3.91	117.49	112.19
6	i	1	NAG	C1-O5-C5	3.85	117.41	112.19
6	b	1	NAG	O4-C4-C5	3.70	118.49	109.30
6	c	1	NAG	O4-C4-C5	3.68	118.44	109.30
6	c	1	NAG	C4-C3-C2	-3.53	105.84	111.02
6	j	1	NAG	O4-C4-C5	3.45	117.86	109.30
6	h	1	NAG	O4-C4-C5	3.40	117.75	109.30
6	h	1	NAG	C4-C3-C2	-3.35	106.10	111.02
6	b	1	NAG	C4-C3-C2	-3.23	106.28	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	e	1	NAG	C4-C3-C2	-3.09	106.49	111.02
6	i	2	NAG	C1-O5-C5	3.06	116.34	112.19
6	j	2	NAG	C1-O5-C5	3.02	116.28	112.19
6	e	1	NAG	C1-C2-N2	2.99	115.60	110.49
6	j	1	NAG	C4-C3-C2	-2.98	106.66	111.02
6	g	2	NAG	C2-N2-C7	2.79	126.88	122.90
6	b	1	NAG	C1-C2-N2	2.76	115.20	110.49
6	c	1	NAG	O4-C4-C3	2.75	116.70	110.35
6	e	1	NAG	O4-C4-C3	2.70	116.59	110.35
6	e	1	NAG	O4-C4-C5	2.66	115.91	109.30
6	c	2	NAG	C1-O5-C5	2.65	115.78	112.19
6	e	1	NAG	C1-O5-C5	2.63	115.76	112.19
6	j	1	NAG	O4-C4-C3	2.61	116.37	110.35
6	h	1	NAG	O4-C4-C3	2.56	116.27	110.35
6	e	2	NAG	C1-O5-C5	2.54	115.63	112.19
6	h	1	NAG	C1-C2-N2	2.51	114.78	110.49
6	c	1	NAG	C1-C2-N2	2.51	114.77	110.49
6	h	2	NAG	C1-O5-C5	2.49	115.56	112.19
6	b	1	NAG	O4-C4-C3	2.36	115.81	110.35
6	g	1	NAG	C3-C4-C5	2.34	114.41	110.24
6	g	1	NAG	O4-C4-C3	-2.26	105.13	110.35
6	g	1	NAG	C1-C2-N2	2.24	114.32	110.49
6	f	1	NAG	O5-C5-C6	-2.24	103.69	107.20
6	d	1	NAG	O5-C5-C6	-2.23	103.72	107.20
6	j	1	NAG	C1-C2-N2	2.17	114.19	110.49
6	a	1	NAG	O4-C4-C5	2.14	114.61	109.30

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	a	1	NAG	C3-C2-N2-C7
6	b	2	NAG	C1-C2-N2-C7
6	d	1	NAG	C3-C2-N2-C7
6	g	2	NAG	C3-C2-N2-C7
6	i	1	NAG	C3-C2-N2-C7
6	d	1	NAG	O5-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6
6	j	1	NAG	O5-C5-C6-O6
6	c	2	NAG	C1-C2-N2-C7
6	e	2	NAG	C1-C2-N2-C7
6	d	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

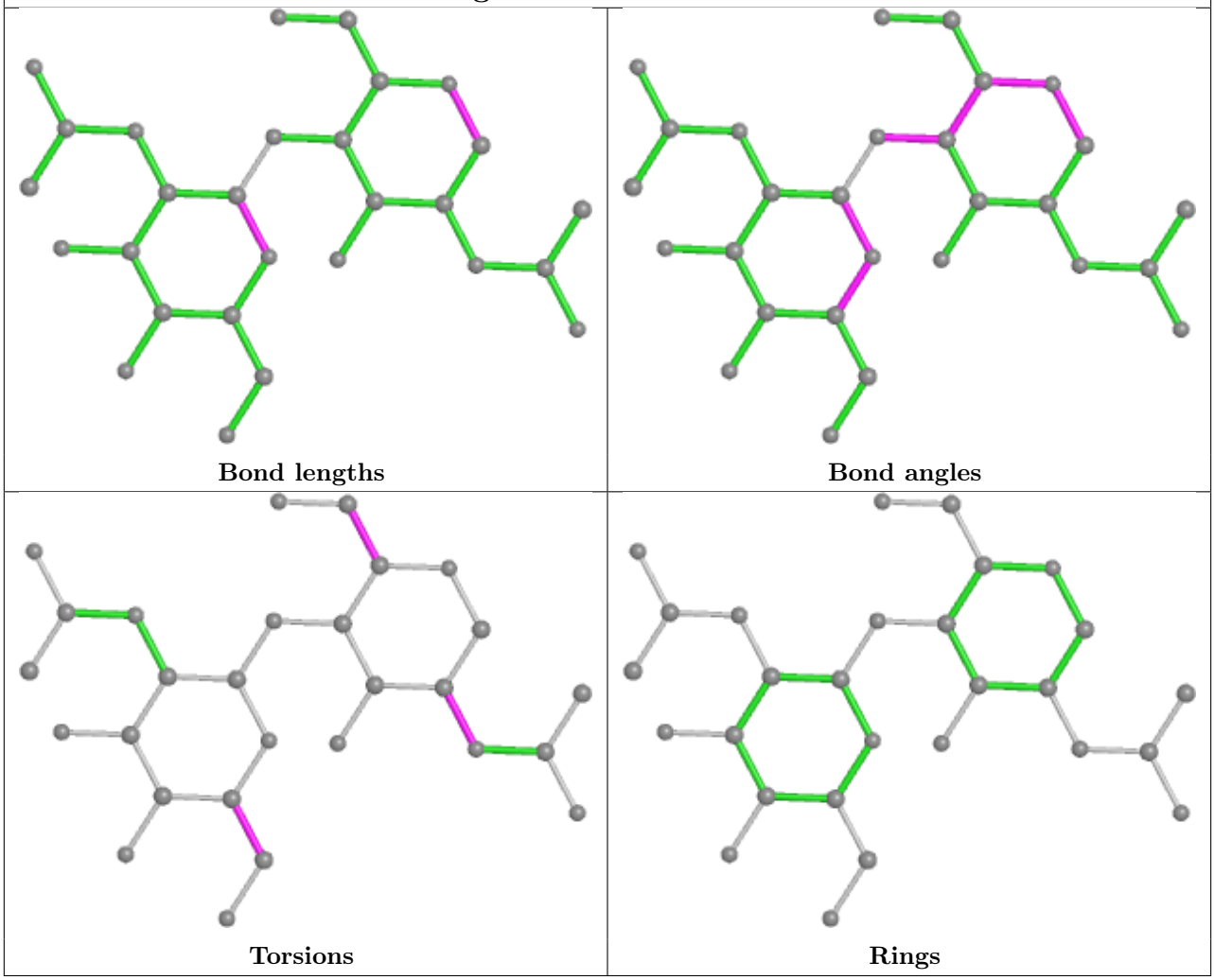
Mol	Chain	Res	Type	Atoms
6	i	1	NAG	O5-C5-C6-O6
6	d	2	NAG	C4-C5-C6-O6
6	h	2	NAG	C4-C5-C6-O6
6	d	1	NAG	C4-C5-C6-O6
6	g	1	NAG	C4-C5-C6-O6
6	c	1	NAG	O5-C5-C6-O6
6	e	1	NAG	O5-C5-C6-O6
6	b	1	NAG	C4-C5-C6-O6
6	h	1	NAG	O5-C5-C6-O6
6	h	2	NAG	O5-C5-C6-O6
6	f	1	NAG	C4-C5-C6-O6
6	j	1	NAG	C4-C5-C6-O6
6	e	1	NAG	C1-C2-N2-C7
6	h	1	NAG	C4-C5-C6-O6
6	b	1	NAG	O5-C5-C6-O6
6	e	1	NAG	C4-C5-C6-O6
6	g	1	NAG	O5-C5-C6-O6
6	g	2	NAG	O5-C5-C6-O6
6	c	1	NAG	C4-C5-C6-O6
6	i	1	NAG	C4-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6
6	j	2	NAG	C1-C2-N2-C7
6	g	2	NAG	C4-C5-C6-O6
6	c	1	NAG	C1-C2-N2-C7
6	j	1	NAG	C1-C2-N2-C7
6	b	2	NAG	O5-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
6	f	1	NAG	C3-C2-N2-C7
6	h	2	NAG	C1-C2-N2-C7
6	f	2	NAG	C4-C5-C6-O6
6	h	1	NAG	C1-C2-N2-C7
6	a	2	NAG	O5-C5-C6-O6
6	b	1	NAG	C1-C2-N2-C7
6	b	2	NAG	C3-C2-N2-C7
6	c	2	NAG	C3-C2-N2-C7
6	e	2	NAG	C3-C2-N2-C7
6	g	1	NAG	C3-C2-N2-C7
6	j	2	NAG	C3-C2-N2-C7
6	g	1	NAG	C1-C2-N2-C7
6	c	2	NAG	O5-C5-C6-O6
6	h	2	NAG	C3-C2-N2-C7

There are no ring outliers.

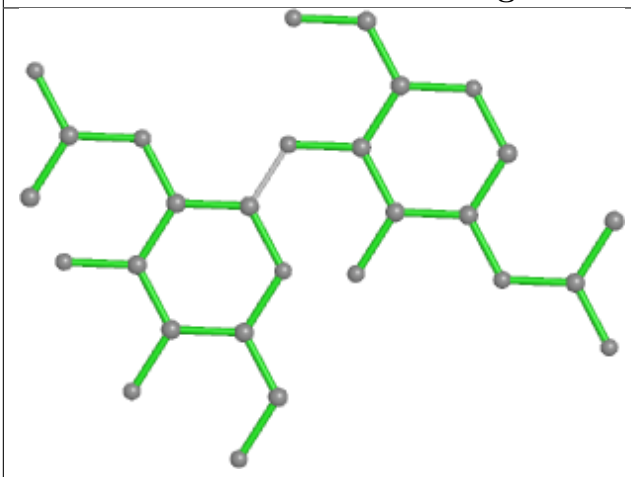
No monomer is involved in short contacts.

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

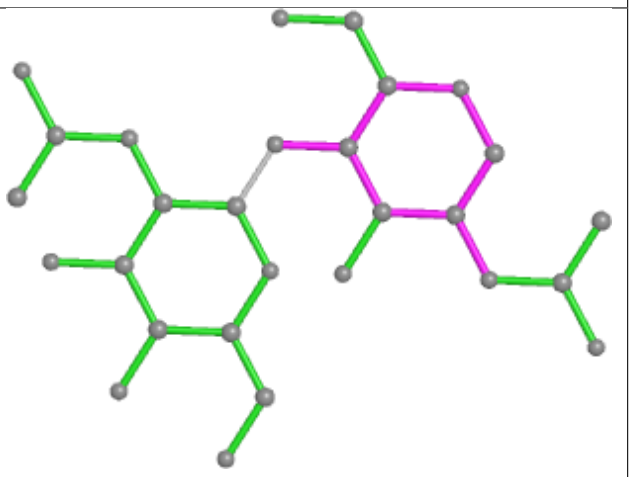
Oligosaccharide Chain a



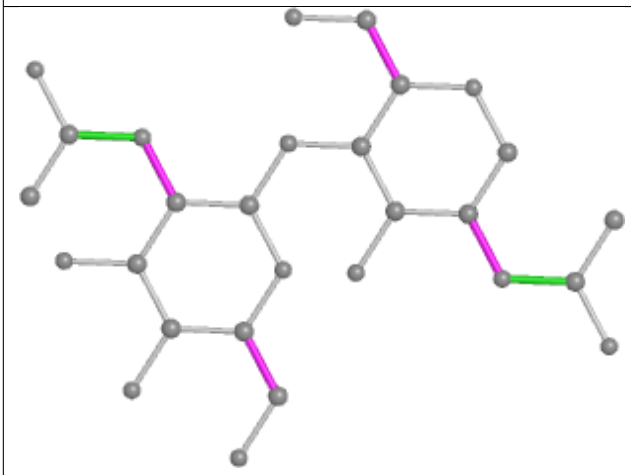
Oligosaccharide Chain b



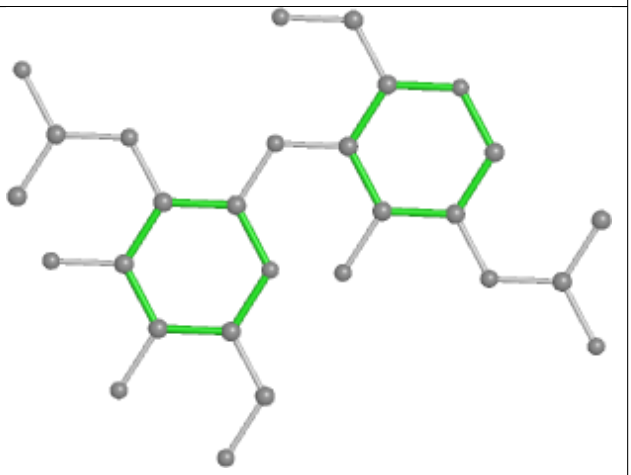
Bond lengths



Bond angles

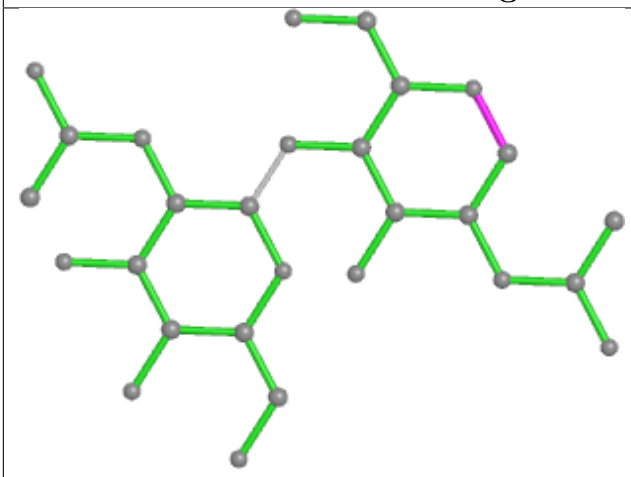


Torsions

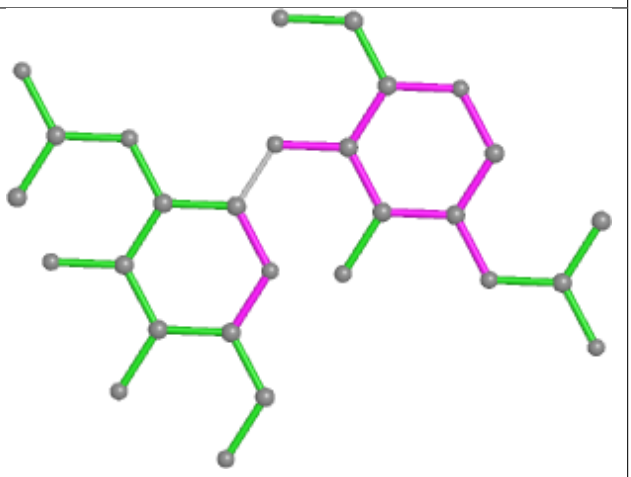


Rings

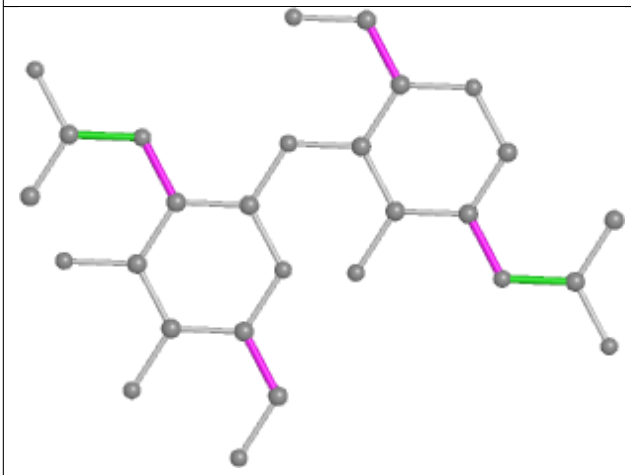
Oligosaccharide Chain c



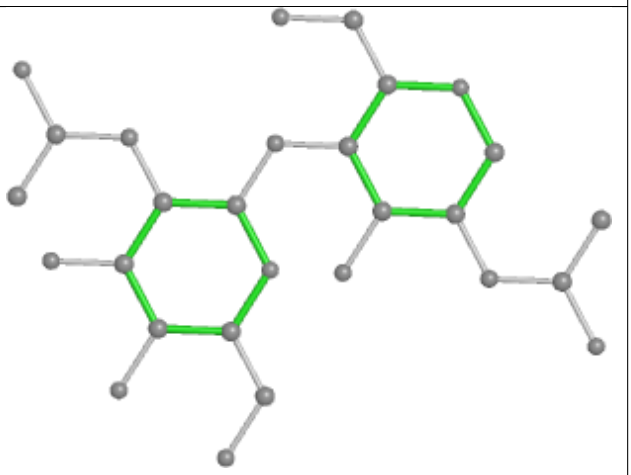
Bond lengths



Bond angles

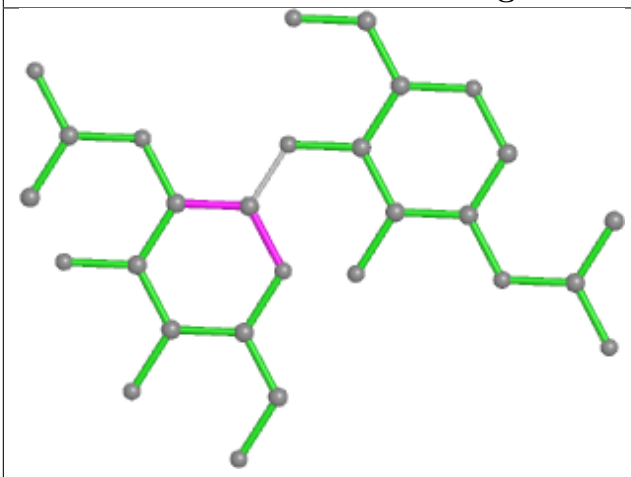


Torsions

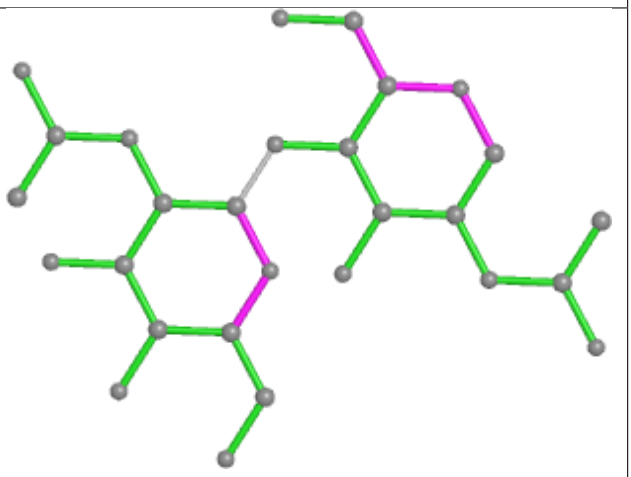


Rings

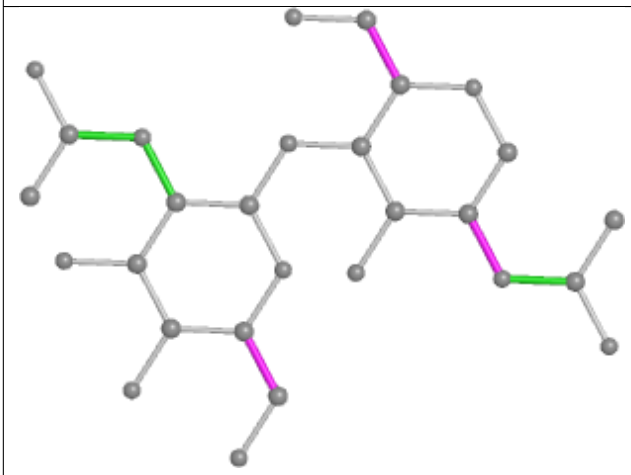
Oligosaccharide Chain d



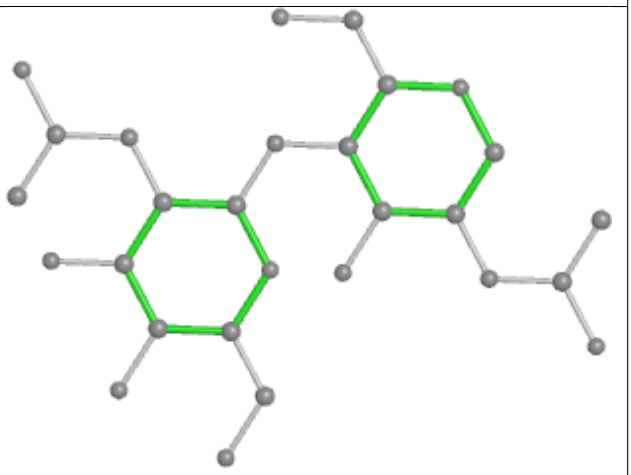
Bond lengths



Bond angles

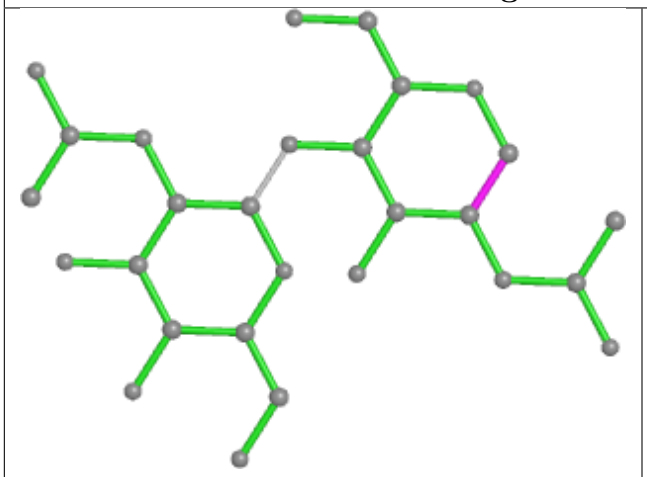


Torsions

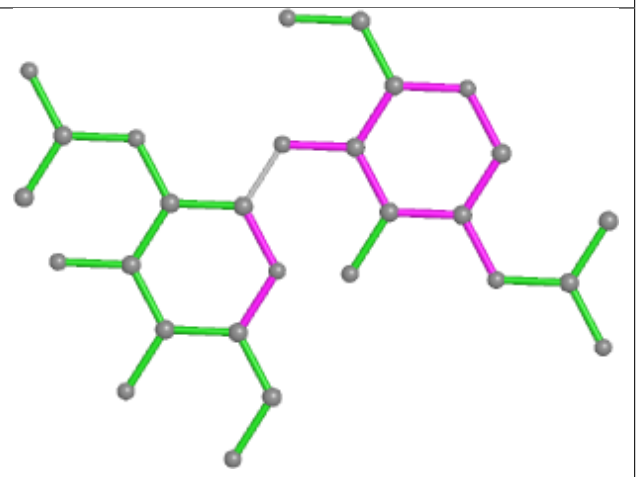


Rings

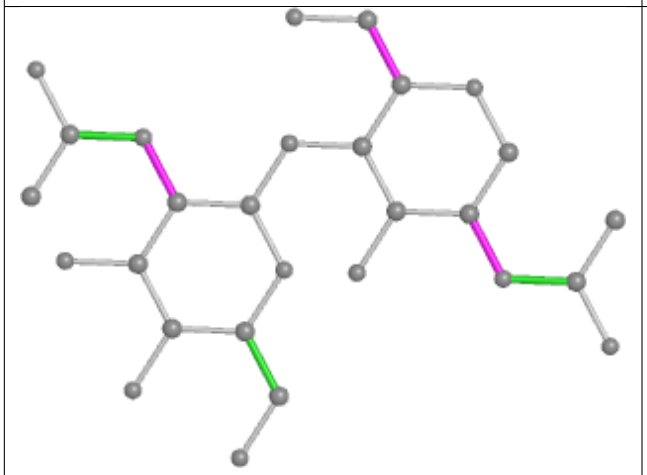
Oligosaccharide Chain e



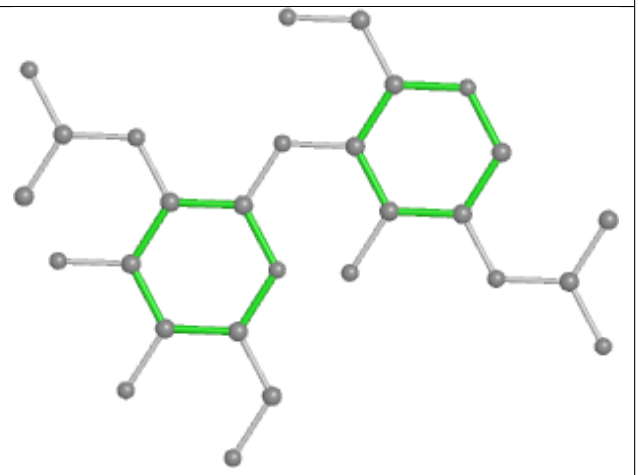
Bond lengths



Bond angles

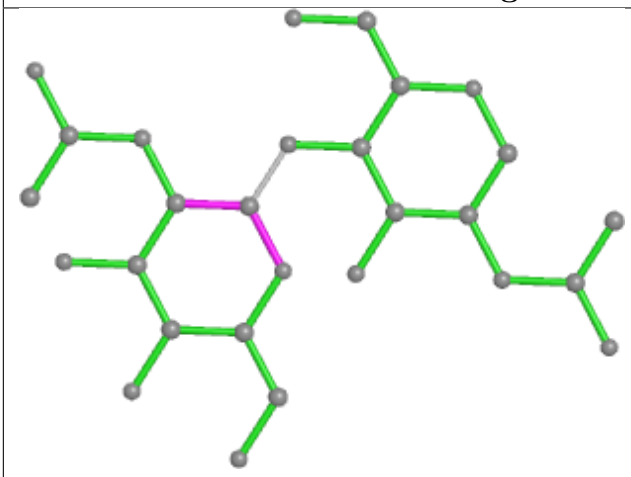


Torsions

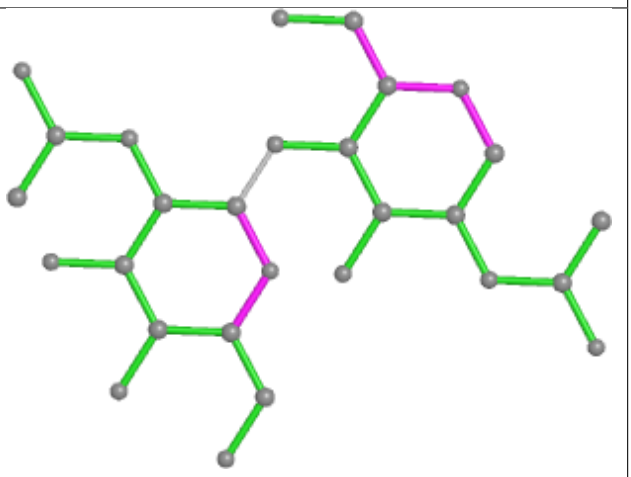


Rings

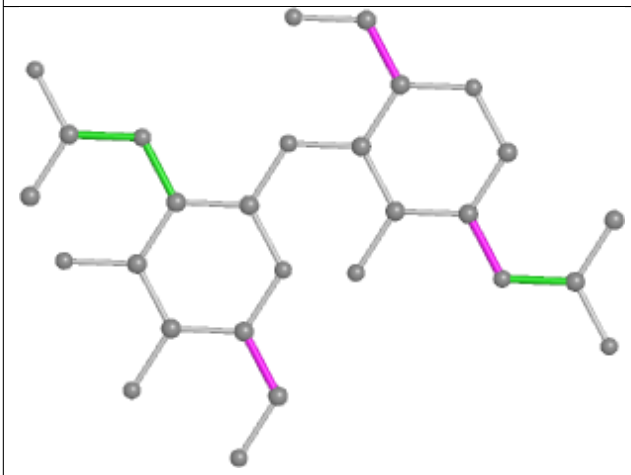
Oligosaccharide Chain f



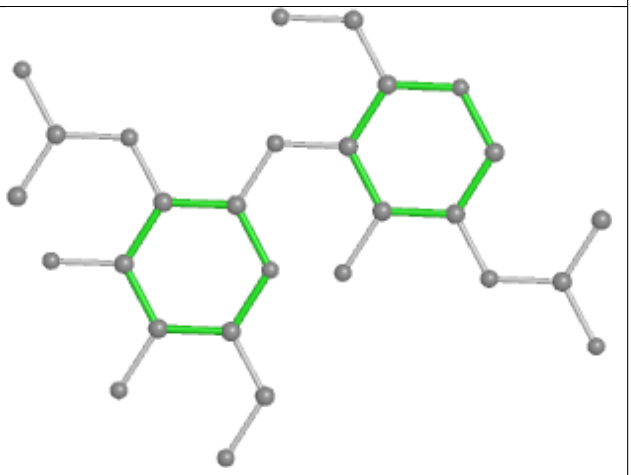
Bond lengths



Bond angles

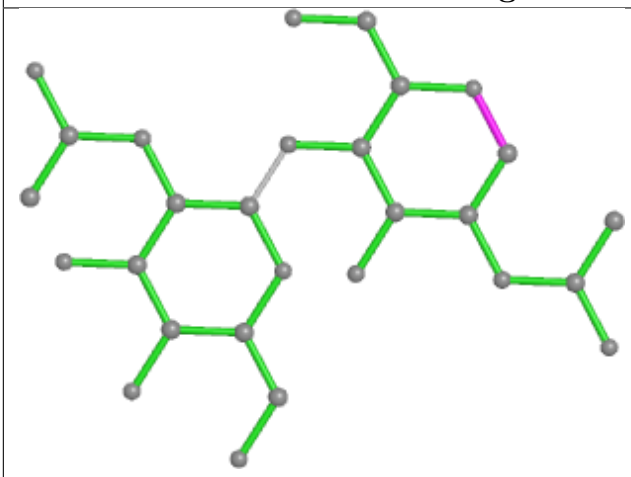


Torsions

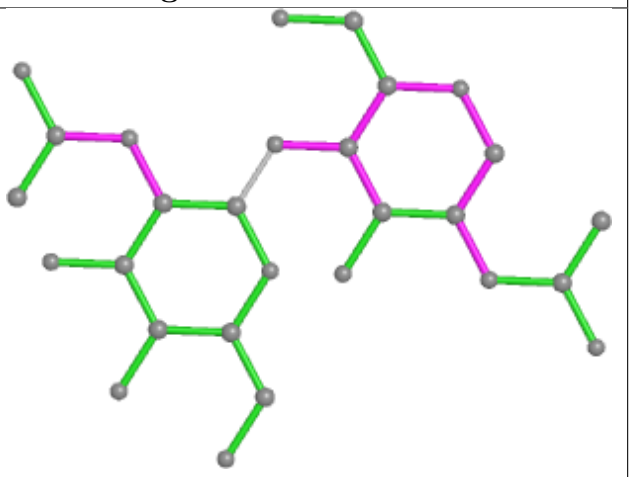


Rings

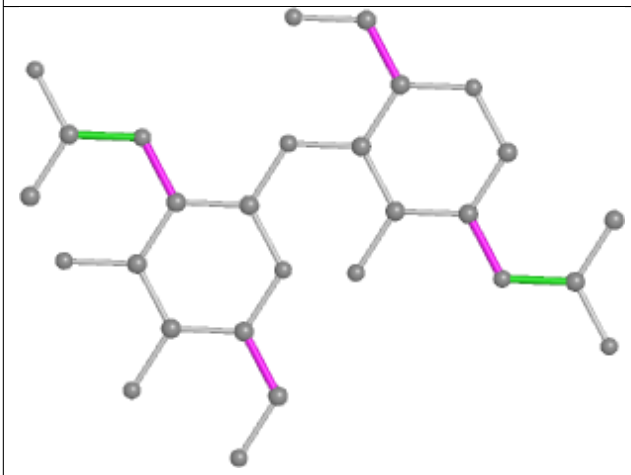
Oligosaccharide Chain g



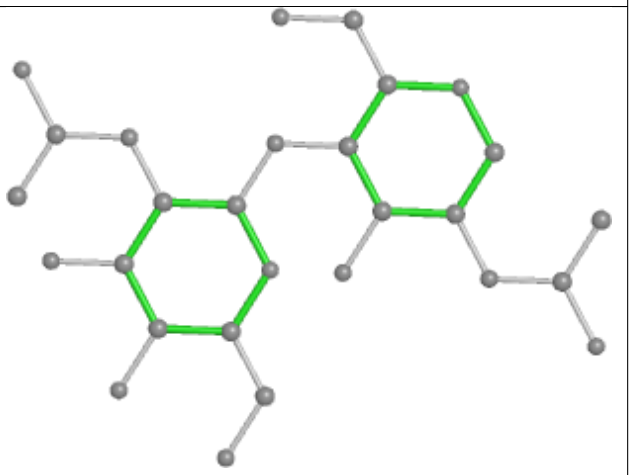
Bond lengths



Bond angles

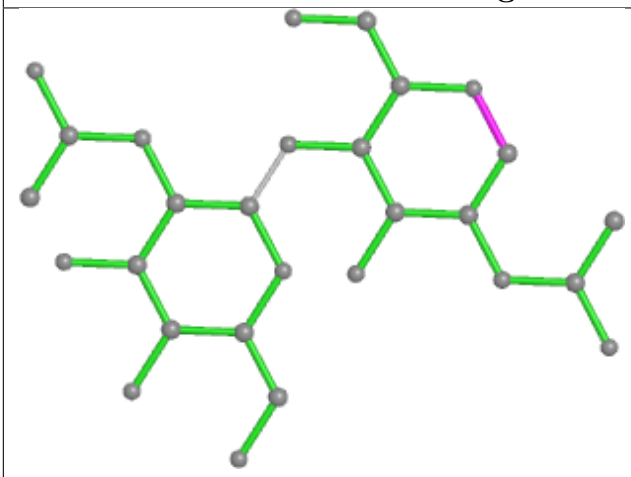


Torsions

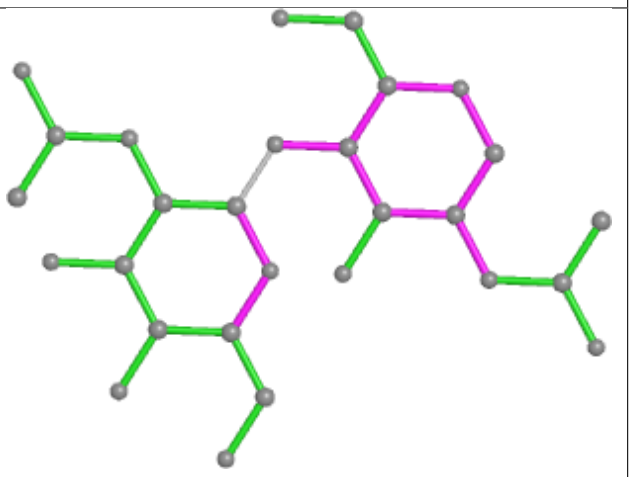


Rings

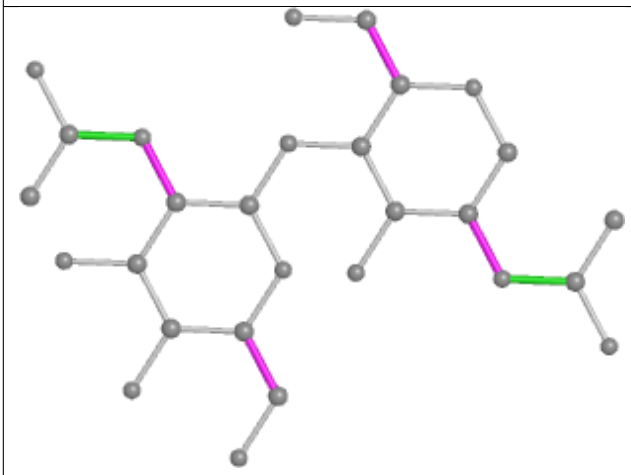
Oligosaccharide Chain h



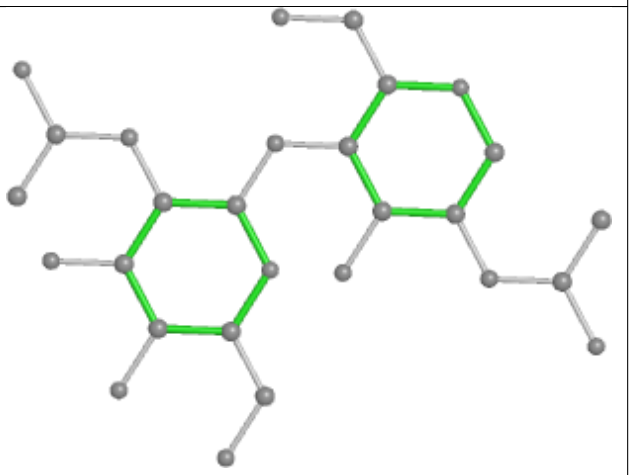
Bond lengths



Bond angles

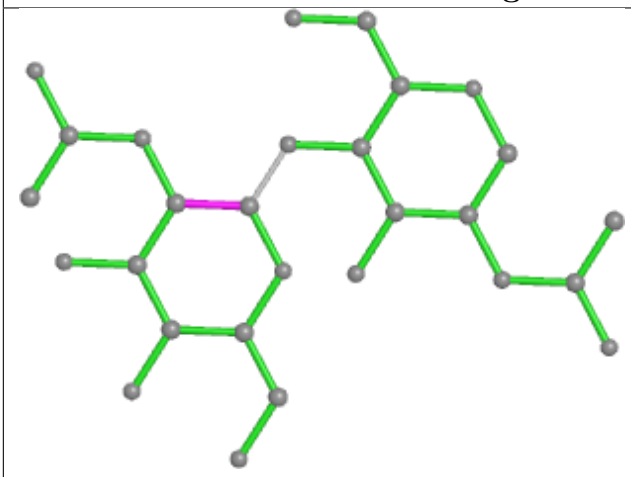


Torsions

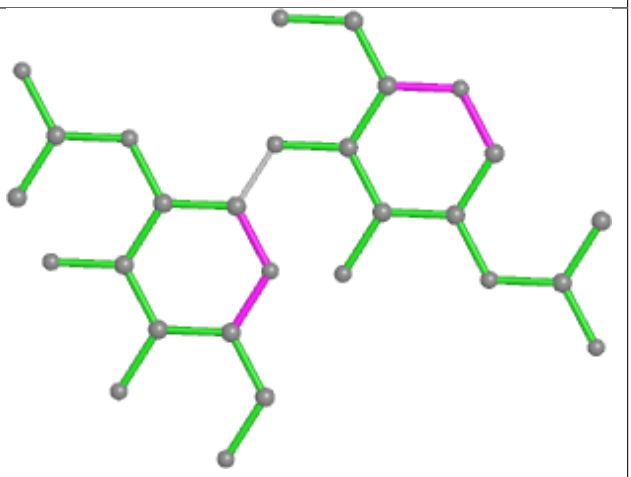


Rings

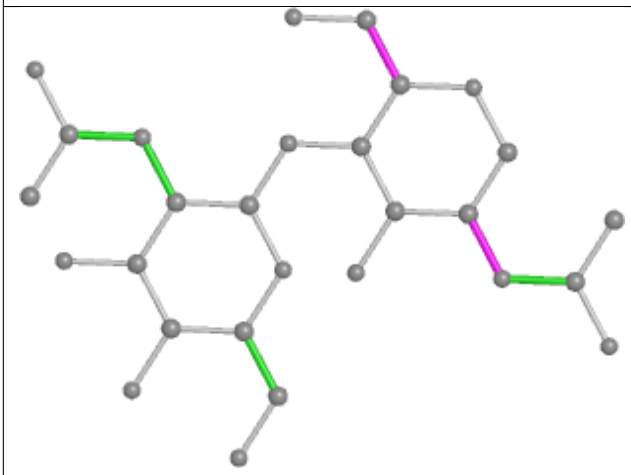
Oligosaccharide Chain i



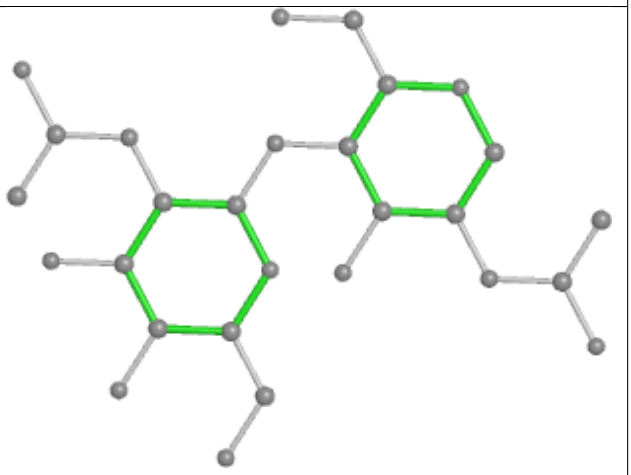
Bond lengths



Bond angles

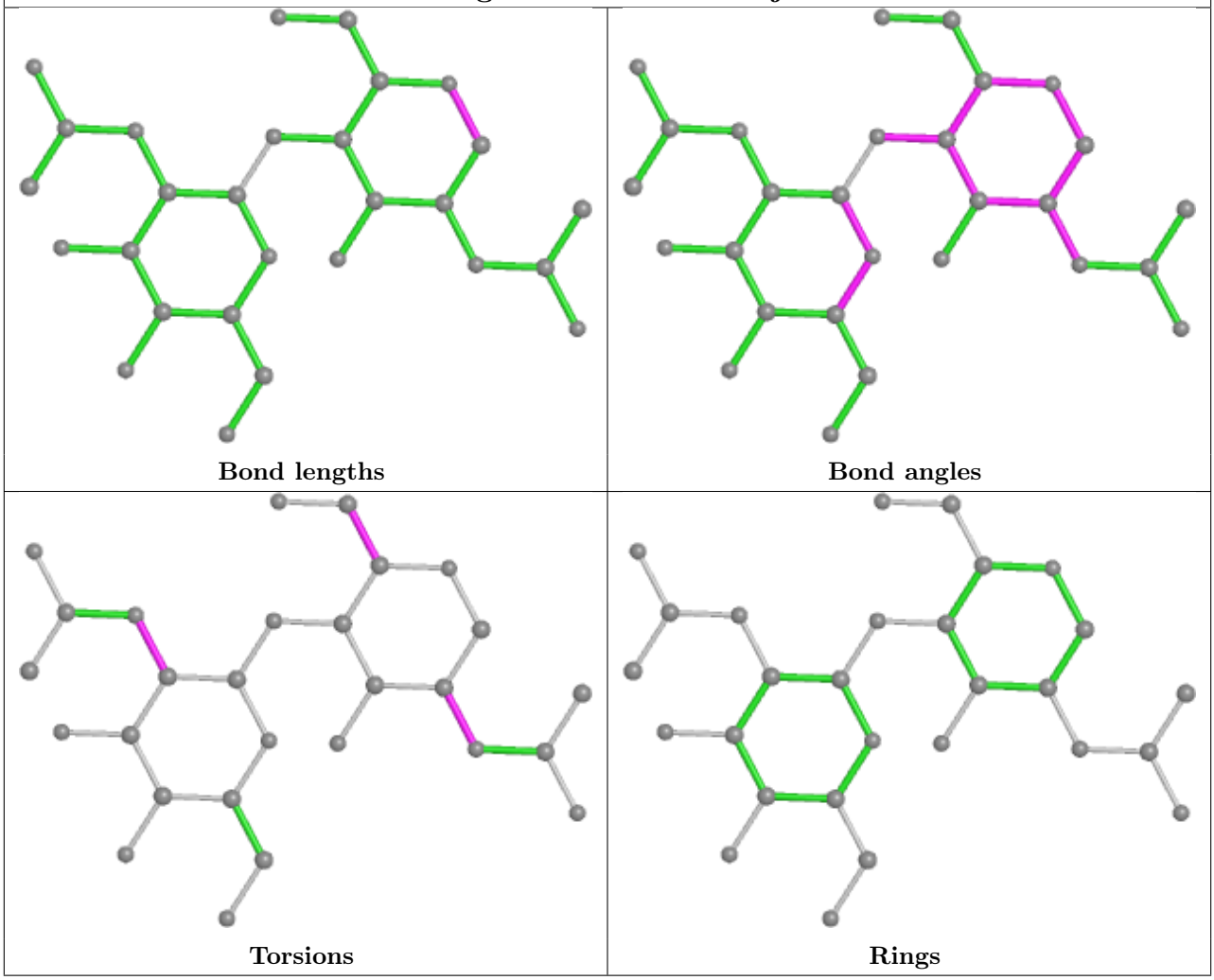


Torsions



Rings

Oligosaccharide Chain j



5.6 Ligand geometry (i)

47 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	OXY	A	202	7	1,1,1	0.10	0	-		
8	OXY	G	202	7	1,1,1	0.11	0	-		
9	NAG	O	1001	5	14,14,15	0.21	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	H	1001	3	14,14,15	0.68	1 (7%)	17,19,21	0.63	0
7	HEM	B	201	2,8	41,50,50	2.04	8 (19%)	45,82,82	2.26	12 (26%)
9	NAG	T	1001	5	14,14,15	0.25	0	17,19,21	0.42	0
9	NAG	2	1001	3	14,14,15	0.26	0	17,19,21	0.53	0
7	HEM	G	201	2,8	41,50,50	2.21	9 (21%)	45,82,82	1.97	12 (26%)
7	HEM	U	201	8,1	41,50,50	2.01	7 (17%)	45,82,82	1.58	5 (11%)
8	OXY	K	202	7	1,1,1	0.08	0	-		
9	NAG	W	1002	3	14,14,15	0.52	0	17,19,21	1.42	1 (5%)
7	HEM	V	201	2,8	41,50,50	2.16	7 (17%)	45,82,82	1.66	5 (11%)
7	HEM	Z	201	8,1	41,50,50	2.01	6 (14%)	45,82,82	1.58	8 (17%)
9	NAG	C	1004	3	14,14,15	1.10	1 (7%)	17,19,21	0.99	1 (5%)
7	HEM	P	201	8,1	41,50,50	1.97	7 (17%)	45,82,82	2.03	9 (20%)
8	OXY	U	202	7	1,1,1	0.13	0	-		
8	OXY	B	202	7	1,1,1	0.11	0	-		
8	OXY	V	202	7	1,1,1	0.14	0	-		
9	NAG	R	1001	3	14,14,15	0.40	0	17,19,21	0.45	0
9	NAG	4	1002	5	14,14,15	0.84	1 (7%)	17,19,21	0.69	0
7	HEM	F	201	8,1	41,50,50	2.04	7 (17%)	45,82,82	1.93	7 (15%)
9	NAG	W	1001	3	14,14,15	0.62	0	17,19,21	0.42	0
8	OXY	1	202	7	1,1,1	0.15	0	-		
7	HEM	1	201	2,8	41,50,50	2.15	8 (19%)	45,82,82	2.15	13 (28%)
9	NAG	E	1002	5	14,14,15	0.75	1 (7%)	17,19,21	1.17	1 (5%)
9	NAG	T	1002	5	14,14,15	0.62	1 (7%)	17,19,21	1.05	1 (5%)
8	OXY	Q	202	7	1,1,1	0.10	0	-		
9	NAG	M	1001	3	14,14,15	0.94	1 (7%)	17,19,21	0.83	1 (5%)
9	NAG	E	1001	5	14,14,15	0.32	0	17,19,21	0.53	0
7	HEM	K	201	8,1	41,50,50	1.95	8 (19%)	45,82,82	2.20	16 (35%)
7	HEM	Q	201	2,8	41,50,50	2.09	9 (21%)	45,82,82	1.98	11 (24%)
7	HEM	L	201	2,8	41,50,50	2.15	9 (21%)	45,82,82	2.73	19 (42%)
9	NAG	4	1001	5	14,14,15	0.19	0	17,19,21	0.49	0
9	NAG	J	1002	5	14,14,15	0.69	1 (7%)	17,19,21	0.45	0
9	NAG	M	1004	3	14,14,15	1.16	1 (7%)	17,19,21	0.93	1 (5%)
7	HEM	A	201	8,1	41,50,50	1.90	6 (14%)	45,82,82	1.75	8 (17%)
9	NAG	J	1001	5	14,14,15	0.39	0	17,19,21	0.53	0
8	OXY	Z	202	7	1,1,1	0.11	0	-		
8	OXY	P	202	7	1,1,1	0.12	0	-		
9	NAG	O	1002	5	14,14,15	0.97	1 (7%)	17,19,21	0.72	0
9	NAG	H	1002	3	14,14,15	0.60	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	Y	1001	5	14,14,15	0.38	0	17,19,21	0.49	0
8	OXY	F	202	7	1,1,1	0.08	0	-		
9	NAG	R	1004	3	14,14,15	0.37	0	17,19,21	0.46	0
8	OXY	L	202	7	1,1,1	0.13	0	-		
9	NAG	C	1001	3	14,14,15	0.44	0	17,19,21	0.57	0
9	NAG	Y	1002	5	14,14,15	0.82	1 (7%)	17,19,21	0.80	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	O	1001	5	-	0/6/23/26	0/1/1/1
9	NAG	H	1001	3	-	1/6/23/26	0/1/1/1
7	HEM	B	201	2,8	-	7/12/54/54	-
9	NAG	T	1001	5	-	2/6/23/26	0/1/1/1
9	NAG	2	1001	3	-	0/6/23/26	0/1/1/1
7	HEM	G	201	2,8	-	5/12/54/54	-
7	HEM	U	201	8,1	-	5/12/54/54	-
9	NAG	W	1002	3	-	3/6/23/26	0/1/1/1
7	HEM	V	201	2,8	-	5/12/54/54	-
7	HEM	Z	201	8,1	-	4/12/54/54	-
9	NAG	C	1004	3	-	0/6/23/26	0/1/1/1
7	HEM	P	201	8,1	-	5/12/54/54	-
9	NAG	R	1001	3	-	1/6/23/26	0/1/1/1
9	NAG	4	1002	5	-	2/6/23/26	0/1/1/1
7	HEM	F	201	8,1	-	3/12/54/54	-
9	NAG	W	1001	3	-	2/6/23/26	0/1/1/1
7	HEM	1	201	2,8	-	8/12/54/54	-
9	NAG	E	1002	5	-	1/6/23/26	0/1/1/1
9	NAG	T	1002	5	-	1/6/23/26	0/1/1/1
9	NAG	M	1001	3	-	2/6/23/26	0/1/1/1
9	NAG	E	1001	5	-	0/6/23/26	0/1/1/1
7	HEM	K	201	8,1	-	3/12/54/54	-
7	HEM	Q	201	2,8	-	5/12/54/54	-
7	HEM	L	201	2,8	-	10/12/54/54	-
9	NAG	4	1001	5	-	0/6/23/26	0/1/1/1
9	NAG	J	1002	5	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	M	1004	3	-	0/6/23/26	0/1/1/1
7	HEM	A	201	8,1	-	5/12/54/54	-
9	NAG	J	1001	5	-	2/6/23/26	0/1/1/1
9	NAG	Y	1001	5	-	2/6/23/26	0/1/1/1
9	NAG	O	1002	5	-	2/6/23/26	0/1/1/1
9	NAG	H	1002	3	-	1/6/23/26	0/1/1/1
9	NAG	R	1004	3	-	0/6/23/26	0/1/1/1
9	NAG	C	1001	3	-	2/6/23/26	0/1/1/1
9	NAG	Y	1002	5	-	1/6/23/26	0/1/1/1

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	201	HEM	C3D-C2D	8.81	1.55	1.36
7	U	201	HEM	C3D-C2D	8.35	1.54	1.36
7	1	201	HEM	C3D-C2D	8.30	1.54	1.36
7	Z	201	HEM	C3D-C2D	8.20	1.54	1.36
7	F	201	HEM	C3D-C2D	8.14	1.54	1.36
7	P	201	HEM	C3D-C2D	7.99	1.53	1.36
7	A	201	HEM	C3D-C2D	7.85	1.53	1.36
7	Q	201	HEM	C3D-C2D	7.78	1.53	1.36
7	L	201	HEM	C3D-C2D	7.75	1.53	1.36
7	G	201	HEM	C3D-C2D	7.59	1.52	1.36
7	B	201	HEM	C3D-C2D	7.54	1.52	1.36
7	K	201	HEM	C3D-C2D	7.25	1.52	1.36
7	G	201	HEM	C3C-C2C	-6.58	1.31	1.40
7	Q	201	HEM	C3C-C2C	-6.15	1.31	1.40
7	V	201	HEM	C3C-C2C	-5.91	1.32	1.40
7	1	201	HEM	C3C-C2C	-5.84	1.32	1.40
7	B	201	HEM	C3C-C2C	-5.73	1.32	1.40
7	L	201	HEM	C3C-C2C	-5.23	1.33	1.40
7	L	201	HEM	FE-NB	4.90	2.21	1.96
7	K	201	HEM	FE-ND	4.64	2.19	1.96
7	A	201	HEM	C3C-C2C	-4.64	1.33	1.40
7	G	201	HEM	FE-NB	4.53	2.19	1.96
7	F	201	HEM	C3C-C2C	-4.42	1.34	1.40
7	V	201	HEM	FE-NB	4.31	2.18	1.96
7	K	201	HEM	C3C-C2C	-4.29	1.34	1.40
7	P	201	HEM	C3C-C2C	-4.10	1.34	1.40
7	Z	201	HEM	C3C-C2C	-4.04	1.34	1.40
7	U	201	HEM	C3C-C2C	-4.04	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	201	HEM	FE-NB	4.01	2.16	1.96
7	Z	201	HEM	C3C-CAC	3.92	1.55	1.47
9	M	1004	NAG	O5-C1	3.91	1.50	1.43
7	F	201	HEM	FE-ND	3.84	2.15	1.96
7	F	201	HEM	C3C-CAC	3.82	1.55	1.47
9	C	1004	NAG	O5-C1	3.77	1.49	1.43
7	B	201	HEM	FE-NB	3.73	2.15	1.96
7	U	201	HEM	C3C-CAC	3.71	1.55	1.47
7	P	201	HEM	C3C-CAC	3.63	1.55	1.47
7	1	201	HEM	FE-NB	3.58	2.14	1.96
9	O	1002	NAG	O5-C1	-3.47	1.38	1.43
7	U	201	HEM	CAB-C3B	3.46	1.56	1.47
7	P	201	HEM	FE-ND	3.28	2.13	1.96
9	M	1001	NAG	O5-C1	-3.24	1.38	1.43
7	G	201	HEM	FE-ND	3.14	2.12	1.96
7	1	201	HEM	CAA-C2A	3.12	1.56	1.52
7	G	201	HEM	CAA-C2A	3.10	1.56	1.52
7	Z	201	HEM	FE-ND	3.10	2.12	1.96
7	K	201	HEM	CAA-C2A	3.08	1.56	1.52
7	F	201	HEM	CAB-C3B	3.07	1.55	1.47
7	Z	201	HEM	CAB-C3B	3.00	1.55	1.47
7	F	201	HEM	CAA-C2A	2.96	1.56	1.52
7	L	201	HEM	FE-ND	2.92	2.11	1.96
7	P	201	HEM	CAA-C2A	2.92	1.56	1.52
9	4	1002	NAG	O5-C1	-2.90	1.39	1.43
7	B	201	HEM	C3C-CAC	2.85	1.53	1.47
7	K	201	HEM	C3C-CAC	2.83	1.53	1.47
7	A	201	HEM	CAB-C3B	2.83	1.55	1.47
7	1	201	HEM	C3C-CAC	2.80	1.53	1.47
7	L	201	HEM	CAB-C3B	2.80	1.55	1.47
7	L	201	HEM	C3C-CAC	2.77	1.53	1.47
9	Y	1002	NAG	O5-C1	-2.76	1.39	1.43
7	P	201	HEM	CAB-C3B	2.73	1.54	1.47
7	A	201	HEM	C3C-CAC	2.72	1.53	1.47
7	A	201	HEM	FE-ND	2.72	2.10	1.96
7	V	201	HEM	C3C-CAC	2.70	1.53	1.47
7	1	201	HEM	C3B-C2B	-2.69	1.31	1.37
7	Q	201	HEM	C3B-C2B	-2.66	1.31	1.37
7	L	201	HEM	CAA-C2A	2.60	1.55	1.52
7	G	201	HEM	C3C-CAC	2.60	1.53	1.47
7	K	201	HEM	CAB-C3B	2.57	1.54	1.47
7	Q	201	HEM	C3C-CAC	2.55	1.53	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	201	HEM	CAB-C3B	2.55	1.54	1.47
9	E	1002	NAG	O5-C1	-2.51	1.39	1.43
7	B	201	HEM	CAB-C3B	2.43	1.54	1.47
7	L	201	HEM	CMD-C2D	2.43	1.55	1.50
7	G	201	HEM	CAB-C3B	2.43	1.54	1.47
9	J	1002	NAG	O5-C1	-2.42	1.39	1.43
7	K	201	HEM	C3B-C2B	-2.35	1.32	1.37
7	U	201	HEM	FE-NB	2.34	2.08	1.96
7	1	201	HEM	CAB-C3B	2.34	1.53	1.47
7	G	201	HEM	C3B-C2B	-2.32	1.32	1.37
7	Q	201	HEM	CAB-C3B	2.29	1.53	1.47
7	L	201	HEM	C3B-C2B	-2.26	1.32	1.37
7	B	201	HEM	CMD-C2D	2.26	1.55	1.50
7	G	201	HEM	CMD-C2D	2.23	1.55	1.50
7	B	201	HEM	C3B-C2B	-2.23	1.32	1.37
7	V	201	HEM	CMB-C2B	2.19	1.55	1.50
7	V	201	HEM	CMD-C2D	2.18	1.55	1.50
7	B	201	HEM	CHC-C4B	-2.17	1.34	1.41
7	Z	201	HEM	CMD-C2D	2.16	1.55	1.50
7	U	201	HEM	FE-ND	2.16	2.07	1.96
7	K	201	HEM	CMD-C2D	2.12	1.55	1.50
9	H	1001	NAG	O5-C1	2.12	1.47	1.43
7	F	201	HEM	CMD-C2D	2.12	1.55	1.50
7	A	201	HEM	CMD-C2D	2.12	1.55	1.50
7	U	201	HEM	CMD-C2D	2.10	1.55	1.50
9	T	1002	NAG	O5-C1	-2.09	1.40	1.43
7	Q	201	HEM	CMD-C2D	2.07	1.55	1.50
7	Q	201	HEM	CAA-C2A	2.06	1.55	1.52
7	1	201	HEM	CMD-C2D	2.04	1.55	1.50
7	Q	201	HEM	CMB-C2B	2.04	1.55	1.50
7	P	201	HEM	FE-NB	2.01	2.06	1.96

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	201	HEM	C4C-CHD-C1D	8.43	133.68	122.56
7	L	201	HEM	C4D-ND-C1D	7.51	112.83	105.07
7	P	201	HEM	C4C-CHD-C1D	6.99	131.78	122.56
7	B	201	HEM	C4D-ND-C1D	6.56	111.85	105.07
7	B	201	HEM	C4C-CHD-C1D	6.50	131.14	122.56
7	1	201	HEM	C4D-ND-C1D	6.42	111.70	105.07
7	P	201	HEM	C4D-ND-C1D	6.36	111.65	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	V	201	HEM	C4D-ND-C1D	6.31	111.59	105.07
7	1	201	HEM	C4C-CHD-C1D	6.20	130.74	122.56
7	F	201	HEM	C4D-ND-C1D	6.16	111.44	105.07
7	Q	201	HEM	C4C-CHD-C1D	6.08	130.58	122.56
7	F	201	HEM	C4C-CHD-C1D	5.75	130.15	122.56
7	A	201	HEM	C4D-ND-C1D	5.71	110.97	105.07
7	U	201	HEM	C4D-ND-C1D	5.64	110.90	105.07
7	K	201	HEM	C4C-CHD-C1D	5.60	129.94	122.56
7	G	201	HEM	C4C-CHD-C1D	5.54	129.87	122.56
7	K	201	HEM	C4D-ND-C1D	5.46	110.72	105.07
7	G	201	HEM	C4D-ND-C1D	5.23	110.47	105.07
7	Q	201	HEM	C4D-ND-C1D	5.19	110.44	105.07
7	Z	201	HEM	C4D-ND-C1D	5.09	110.33	105.07
7	A	201	HEM	C4C-CHD-C1D	4.93	129.06	122.56
7	L	201	HEM	CAD-C3D-C4D	4.90	133.22	124.66
7	L	201	HEM	CAD-CBD-CGD	-4.88	103.09	113.60
7	Z	201	HEM	C4C-CHD-C1D	4.70	128.76	122.56
7	F	201	HEM	CMA-C3A-C4A	-4.63	121.36	128.46
7	U	201	HEM	C4C-CHD-C1D	4.51	128.51	122.56
7	K	201	HEM	CMA-C3A-C4A	-4.40	121.71	128.46
9	W	1002	NAG	C1-O5-C5	4.38	118.13	112.19
7	B	201	HEM	CAD-CBD-CGD	-4.32	104.31	113.60
7	Q	201	HEM	CAA-CBA-CGA	-4.04	102.45	113.76
7	1	201	HEM	C4A-C3A-C2A	3.92	109.72	107.00
7	P	201	HEM	C4A-C3A-C2A	3.89	109.70	107.00
7	V	201	HEM	C4C-CHD-C1D	3.74	127.50	122.56
9	T	1002	NAG	C2-N2-C7	3.73	128.22	122.90
7	B	201	HEM	CAA-CBA-CGA	-3.73	103.30	113.76
7	F	201	HEM	C4A-C3A-C2A	3.69	109.56	107.00
9	C	1004	NAG	C1-O5-C5	3.64	117.13	112.19
9	E	1002	NAG	C2-N2-C7	3.47	127.84	122.90
7	L	201	HEM	C3B-C2B-C1B	3.44	109.04	106.49
7	L	201	HEM	C4A-C3A-C2A	3.40	109.36	107.00
9	M	1004	NAG	C1-O5-C5	3.31	116.68	112.19
7	K	201	HEM	C4A-C3A-C2A	3.28	109.28	107.00
7	P	201	HEM	C1B-NB-C4B	3.26	108.44	105.07
7	L	201	HEM	CHD-C1D-ND	3.23	127.94	124.43
7	B	201	HEM	CMD-C2D-C1D	3.22	129.95	125.04
7	Q	201	HEM	CHB-C1B-NB	3.22	128.36	124.38
7	1	201	HEM	CHD-C1D-ND	3.21	127.92	124.43
7	Z	201	HEM	CBA-CAA-C2A	-3.20	107.15	112.62
7	K	201	HEM	CMD-C2D-C1D	3.19	129.90	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1	201	HEM	C3B-C2B-C1B	3.18	108.85	106.49
7	L	201	HEM	CHB-C1B-NB	3.18	128.31	124.38
7	L	201	HEM	CAD-C3D-C2D	-3.18	121.95	127.88
7	B	201	HEM	CHB-C1B-NB	3.17	128.30	124.38
7	1	201	HEM	CBA-CAA-C2A	3.14	117.97	112.62
7	K	201	HEM	C1B-NB-C4B	3.13	108.31	105.07
7	B	201	HEM	CAD-C3D-C4D	3.12	130.12	124.66
7	L	201	HEM	CAA-CBA-CGA	-3.11	105.03	113.76
7	G	201	HEM	CBA-CAA-C2A	3.10	117.92	112.62
7	A	201	HEM	CMA-C3A-C4A	-3.10	123.70	128.46
7	G	201	HEM	C2C-C3C-C4C	3.09	109.06	106.90
7	G	201	HEM	CMD-C2D-C1D	3.06	129.70	125.04
7	L	201	HEM	CAA-C2A-C3A	-3.04	118.52	127.25
7	B	201	HEM	C3B-C2B-C1B	3.03	108.74	106.49
7	K	201	HEM	C3B-C2B-C1B	3.02	108.72	106.49
7	F	201	HEM	C1B-NB-C4B	3.01	108.18	105.07
7	V	201	HEM	CHD-C1D-ND	2.97	127.66	124.43
7	B	201	HEM	CAA-C2A-C3A	-2.89	118.95	127.25
7	G	201	HEM	C4A-C3A-C2A	2.88	109.00	107.00
7	K	201	HEM	C1D-C2D-C3D	-2.87	103.93	106.96
7	P	201	HEM	CMA-C3A-C4A	-2.86	124.06	128.46
7	K	201	HEM	CMB-C2B-C1B	2.85	129.38	125.04
7	L	201	HEM	CMD-C2D-C1D	2.84	129.37	125.04
7	Q	201	HEM	CAD-CBD-CGD	-2.81	107.55	113.60
7	B	201	HEM	CHD-C1D-ND	2.77	127.44	124.43
7	V	201	HEM	CAA-CBA-CGA	-2.76	106.02	113.76
7	A	201	HEM	CHC-C4B-NB	2.75	127.42	124.43
7	G	201	HEM	CAD-C3D-C4D	2.75	129.46	124.66
7	F	201	HEM	CHC-C4B-NB	2.72	127.38	124.43
7	G	201	HEM	CAA-CBA-CGA	-2.70	106.18	113.76
7	L	201	HEM	CMA-C3A-C4A	-2.67	124.36	128.46
7	K	201	HEM	CBA-CAA-C2A	2.67	117.18	112.62
7	K	201	HEM	CBD-CAD-C3D	-2.66	105.25	112.63
7	K	201	HEM	CMB-C2B-C3B	-2.62	121.88	128.30
7	B	201	HEM	C2C-C3C-C4C	2.62	108.73	106.90
7	L	201	HEM	CBA-CAA-C2A	2.60	117.05	112.62
7	L	201	HEM	C2C-C3C-C4C	2.59	108.71	106.90
9	M	1001	NAG	C1-O5-C5	-2.57	108.71	112.19
7	1	201	HEM	CAD-C3D-C4D	2.56	129.12	124.66
7	Q	201	HEM	C2C-C3C-C4C	2.55	108.68	106.90
7	Q	201	HEM	CBD-CAD-C3D	-2.53	105.61	112.63
7	1	201	HEM	CAD-CBD-CGD	-2.52	108.19	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	201	HEM	CAD-CBD-CGD	-2.48	108.26	113.60
7	1	201	HEM	CMB-C2B-C1B	2.47	128.80	125.04
7	A	201	HEM	O1A-CGA-CBA	-2.46	115.17	123.08
7	Q	201	HEM	CAD-C3D-C4D	2.45	128.93	124.66
7	1	201	HEM	CMB-C2B-C3B	-2.43	122.34	128.30
7	U	201	HEM	CMC-C2C-C3C	2.40	129.17	124.68
7	1	201	HEM	CAA-C2A-C3A	-2.40	120.34	127.25
7	Z	201	HEM	C4A-C3A-C2A	2.33	108.62	107.00
7	K	201	HEM	CHC-C4B-NB	2.32	126.95	124.43
7	L	201	HEM	O1D-CGD-CBD	-2.30	115.69	123.08
7	G	201	HEM	CAD-CBD-CGD	-2.29	108.67	113.60
7	P	201	HEM	CHD-C1D-ND	2.28	126.91	124.43
7	G	201	HEM	CHC-C4B-C3B	2.28	128.06	124.57
7	Q	201	HEM	CMD-C2D-C1D	2.27	128.49	125.04
7	1	201	HEM	CAA-CBA-CGA	-2.23	107.50	113.76
7	G	201	HEM	C3B-C2B-C1B	2.23	108.14	106.49
7	Q	201	HEM	C3B-C2B-C1B	2.21	108.13	106.49
7	V	201	HEM	CHA-C4D-ND	2.21	127.11	124.38
7	Q	201	HEM	CHD-C1D-ND	2.20	126.82	124.43
7	F	201	HEM	CMA-C3A-C2A	2.19	129.08	124.94
7	U	201	HEM	CBA-CAA-C2A	-2.18	108.89	112.62
7	Z	201	HEM	CAA-CBA-CGA	-2.18	107.64	113.76
7	Z	201	HEM	CMC-C2C-C3C	2.18	128.76	124.68
7	L	201	HEM	CAB-C3B-C2B	-2.17	121.44	128.60
7	1	201	HEM	C2C-C3C-C4C	2.17	108.41	106.90
7	K	201	HEM	CMA-C3A-C2A	2.16	129.02	124.94
7	L	201	HEM	C2D-C1D-ND	-2.15	107.30	109.88
7	A	201	HEM	CAA-CBA-CGA	-2.15	107.73	113.76
7	B	201	HEM	C4A-C3A-C2A	2.15	108.49	107.00
7	A	201	HEM	CMC-C2C-C3C	2.13	128.66	124.68
7	P	201	HEM	CBA-CAA-C2A	2.10	116.20	112.62
7	P	201	HEM	CAD-CBD-CGD	-2.09	109.10	113.60
7	K	201	HEM	CHA-C4D-ND	2.09	126.97	124.38
7	Z	201	HEM	O1A-CGA-CBA	-2.08	116.39	123.08
7	U	201	HEM	O2D-CGD-CBD	2.08	120.70	114.03
7	Z	201	HEM	C1D-C2D-C3D	-2.08	104.77	106.96
7	G	201	HEM	C1B-NB-C4B	2.07	107.21	105.07
7	P	201	HEM	O1A-CGA-CBA	-2.06	116.47	123.08
9	Y	1002	NAG	C1-C2-N2	2.04	113.97	110.49
7	A	201	HEM	C1B-NB-C4B	2.03	107.17	105.07
7	L	201	HEM	O1A-CGA-CBA	-2.02	116.59	123.08

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	201	HEM	C1A-C2A-CAA-CBA
7	B	201	HEM	C3A-C2A-CAA-CBA
7	K	201	HEM	C2A-CAA-CBA-CGA
7	L	201	HEM	C1A-C2A-CAA-CBA
7	L	201	HEM	C3A-C2A-CAA-CBA
7	L	201	HEM	C2A-CAA-CBA-CGA
7	Z	201	HEM	C2D-C3D-CAD-CBD
7	1	201	HEM	C1A-C2A-CAA-CBA
7	1	201	HEM	C3A-C2A-CAA-CBA
7	1	201	HEM	C2A-CAA-CBA-CGA
9	E	1002	NAG	C3-C2-N2-C7
9	M	1001	NAG	C1-C2-N2-C7
9	T	1002	NAG	C3-C2-N2-C7
9	W	1002	NAG	O5-C5-C6-O6
9	J	1001	NAG	O5-C5-C6-O6
7	Z	201	HEM	C4D-C3D-CAD-CBD
9	T	1001	NAG	O5-C5-C6-O6
9	W	1002	NAG	C4-C5-C6-O6
7	A	201	HEM	C2D-C3D-CAD-CBD
9	J	1001	NAG	C4-C5-C6-O6
7	F	201	HEM	C2D-C3D-CAD-CBD
9	W	1001	NAG	O5-C5-C6-O6
7	B	201	HEM	C2A-CAA-CBA-CGA
7	F	201	HEM	C2A-CAA-CBA-CGA
7	P	201	HEM	C2A-CAA-CBA-CGA
7	Z	201	HEM	C2A-CAA-CBA-CGA
7	A	201	HEM	C4D-C3D-CAD-CBD
9	H	1002	NAG	O5-C5-C6-O6
7	Z	201	HEM	C3D-CAD-CBD-CGD
9	H	1001	NAG	O5-C5-C6-O6
9	T	1001	NAG	C4-C5-C6-O6
9	O	1002	NAG	C1-C2-N2-C7
7	F	201	HEM	C4D-C3D-CAD-CBD
9	R	1001	NAG	O5-C5-C6-O6
9	J	1002	NAG	C1-C2-N2-C7
9	4	1002	NAG	C1-C2-N2-C7
9	C	1001	NAG	C4-C5-C6-O6
9	W	1001	NAG	C4-C5-C6-O6
9	W	1002	NAG	C3-C2-N2-C7
9	4	1002	NAG	C3-C2-N2-C7
9	C	1001	NAG	O5-C5-C6-O6
9	Y	1001	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	L	201	HEM	C3D-CAD-CBD-CGD
7	B	201	HEM	C4B-C3B-CAB-CBB
7	G	201	HEM	C4B-C3B-CAB-CBB
7	Q	201	HEM	C4B-C3B-CAB-CBB
7	1	201	HEM	C4B-C3B-CAB-CBB
7	L	201	HEM	C4D-C3D-CAD-CBD
7	A	201	HEM	C2A-CAA-CBA-CGA
7	G	201	HEM	C2A-CAA-CBA-CGA
7	Q	201	HEM	C2A-CAA-CBA-CGA
7	Q	201	HEM	C3A-C2A-CAA-CBA
7	U	201	HEM	C2D-C3D-CAD-CBD
7	P	201	HEM	C2D-C3D-CAD-CBD
7	V	201	HEM	C2D-C3D-CAD-CBD
7	U	201	HEM	C4D-C3D-CAD-CBD
9	M	1001	NAG	C3-C2-N2-C7
9	Y	1002	NAG	C3-C2-N2-C7
9	Y	1001	NAG	O5-C5-C6-O6
7	P	201	HEM	CAD-CBD-CGD-O2D
7	U	201	HEM	C2A-CAA-CBA-CGA
7	P	201	HEM	C4D-C3D-CAD-CBD
7	L	201	HEM	CAA-CBA-CGA-O1A
7	G	201	HEM	CAD-CBD-CGD-O1D
7	U	201	HEM	CAD-CBD-CGD-O1D
7	V	201	HEM	CAD-CBD-CGD-O1D
7	G	201	HEM	CAD-CBD-CGD-O2D
7	L	201	HEM	CAA-CBA-CGA-O2A
7	1	201	HEM	CAA-CBA-CGA-O1A
7	L	201	HEM	CAD-CBD-CGD-O2D
7	V	201	HEM	CAD-CBD-CGD-O2D
7	L	201	HEM	C2D-C3D-CAD-CBD
7	U	201	HEM	CAD-CBD-CGD-O2D
7	1	201	HEM	CAD-CBD-CGD-O1D
7	G	201	HEM	C3D-CAD-CBD-CGD
7	A	201	HEM	CAD-CBD-CGD-O1D
7	L	201	HEM	CAD-CBD-CGD-O1D
7	1	201	HEM	CAD-CBD-CGD-O2D
7	1	201	HEM	CAA-CBA-CGA-O2A
7	V	201	HEM	C4D-C3D-CAD-CBD
7	P	201	HEM	CAD-CBD-CGD-O1D
7	A	201	HEM	CAD-CBD-CGD-O2D
7	K	201	HEM	CAD-CBD-CGD-O2D
7	V	201	HEM	C3D-CAD-CBD-CGD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	Q	201	HEM	CAD-CBD-CGD-O1D
7	B	201	HEM	CAD-CBD-CGD-O1D
7	B	201	HEM	C3D-CAD-CBD-CGD
7	Q	201	HEM	CAD-CBD-CGD-O2D
7	K	201	HEM	CAD-CBD-CGD-O1D
7	B	201	HEM	CAD-CBD-CGD-O2D
9	J	1002	NAG	C3-C2-N2-C7
9	O	1002	NAG	C3-C2-N2-C7

There are no ring outliers.

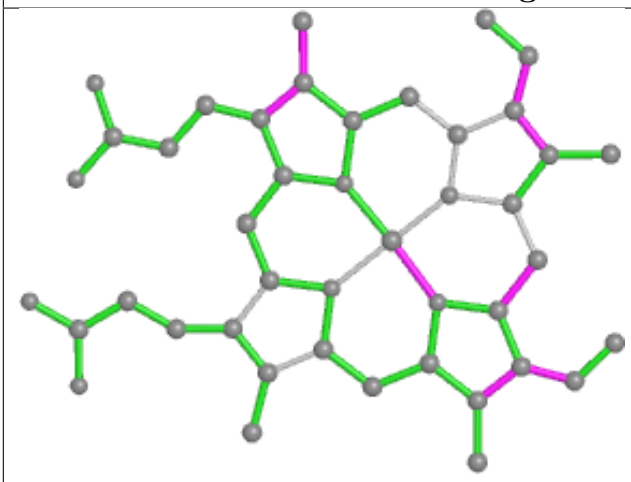
23 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	201	HEM	6	0
7	G	201	HEM	3	0
7	U	201	HEM	4	0
9	W	1002	NAG	1	0
7	V	201	HEM	3	0
7	Z	201	HEM	2	0
7	P	201	HEM	2	0
8	U	202	OXY	1	0
8	V	202	OXY	1	0
9	4	1002	NAG	2	0
7	F	201	HEM	2	0
7	1	201	HEM	6	0
9	E	1002	NAG	1	0
9	T	1002	NAG	1	0
9	M	1001	NAG	1	0
7	K	201	HEM	1	0
7	Q	201	HEM	4	0
7	L	201	HEM	6	0
9	J	1002	NAG	2	0
7	A	201	HEM	1	0
8	Z	202	OXY	1	0
9	O	1002	NAG	1	0
9	Y	1002	NAG	1	0

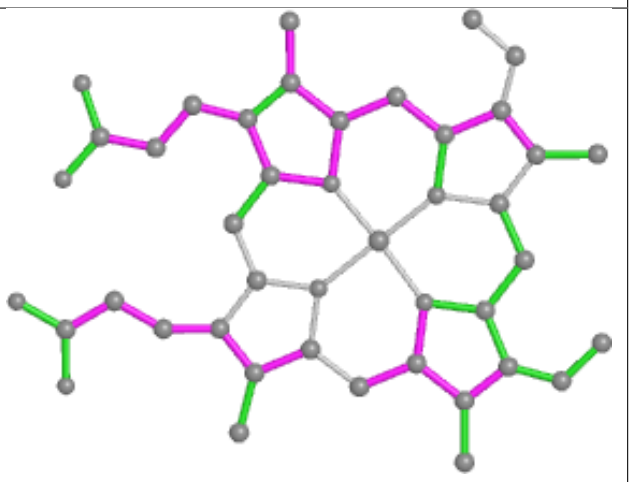
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

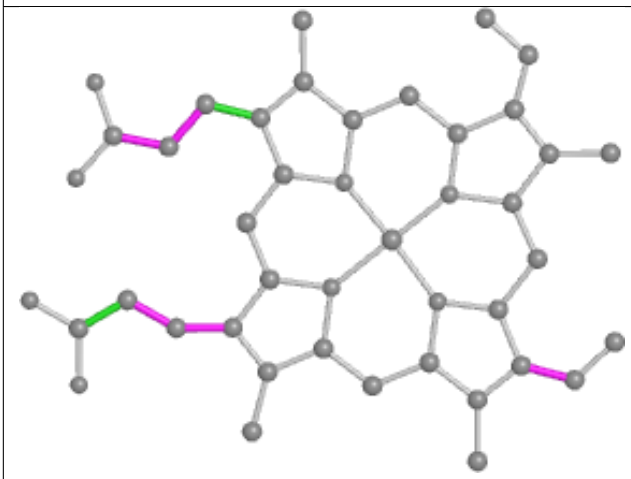
Ligand HEM B 201



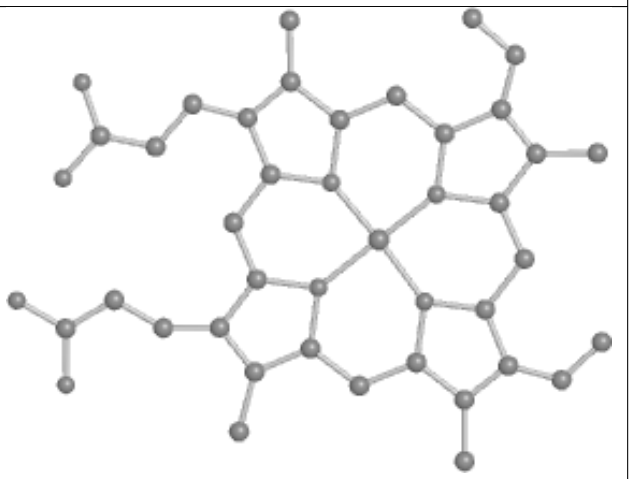
Bond lengths



Bond angles

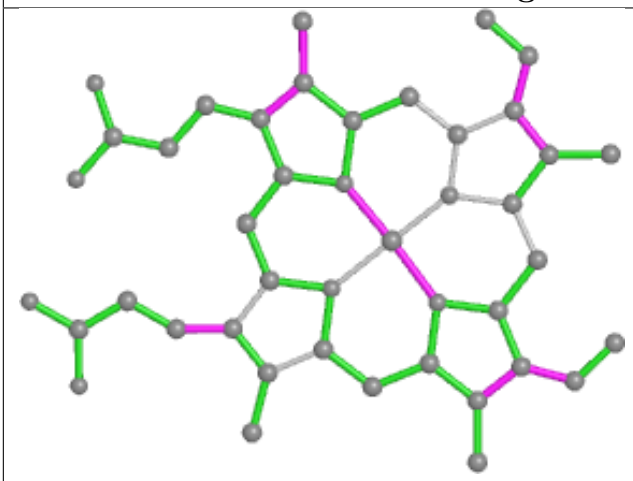


Torsions

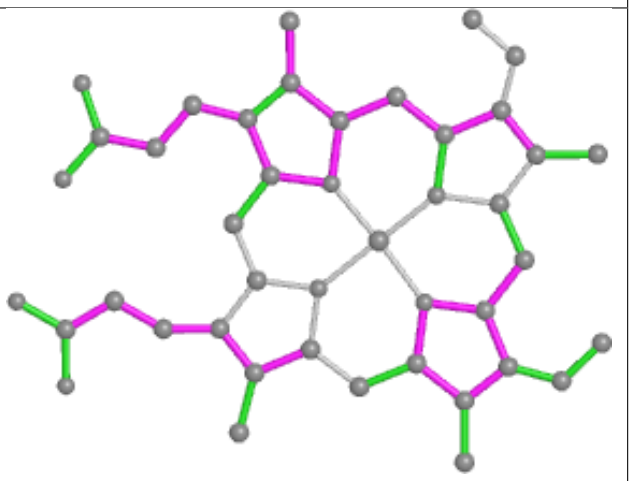


Rings

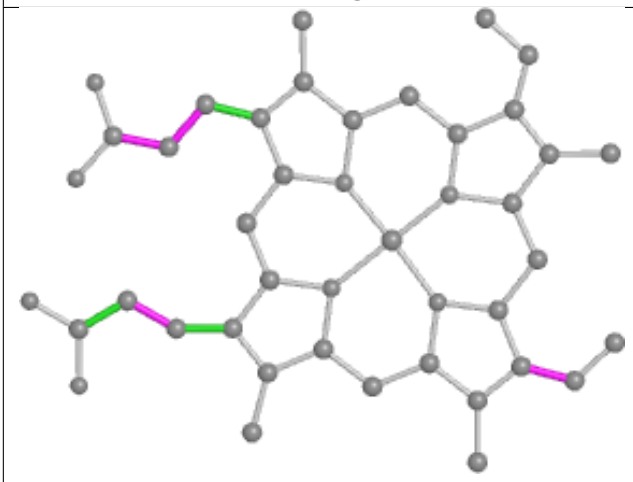
Ligand HEM G 201



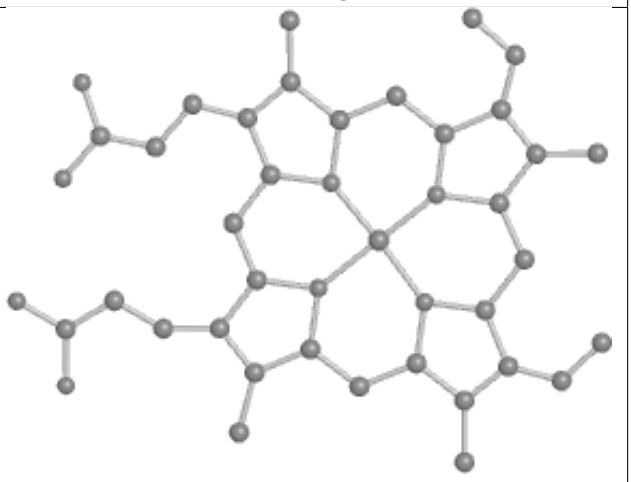
Bond lengths



Bond angles

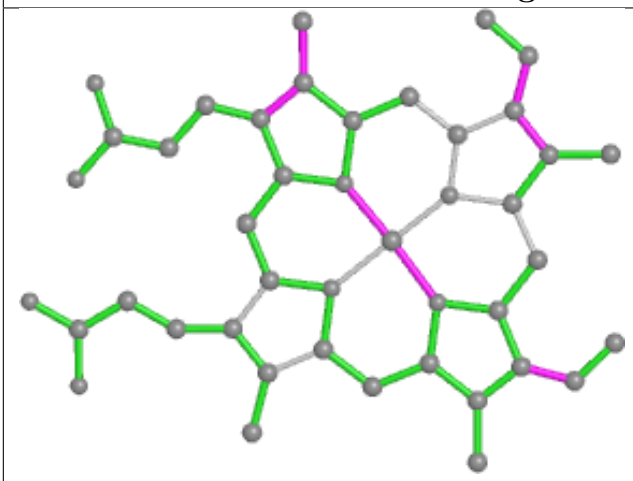


Torsions

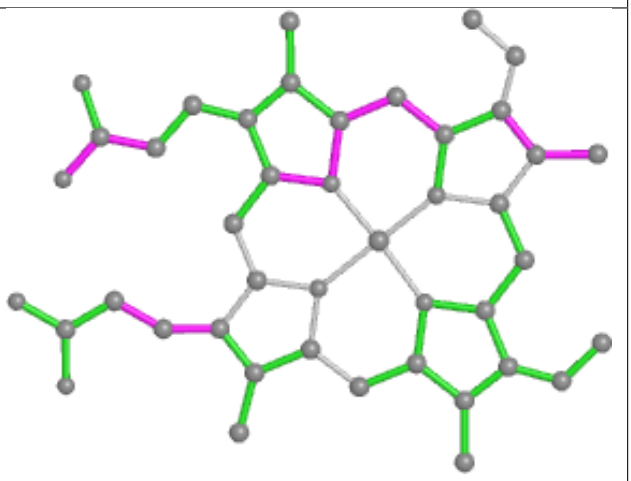


Rings

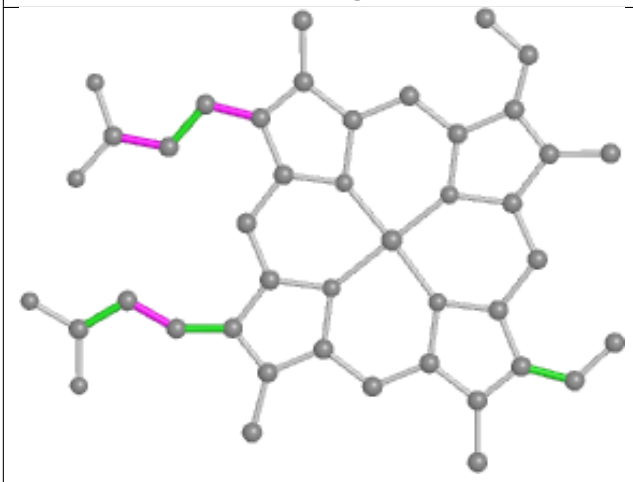
Ligand HEM U 201



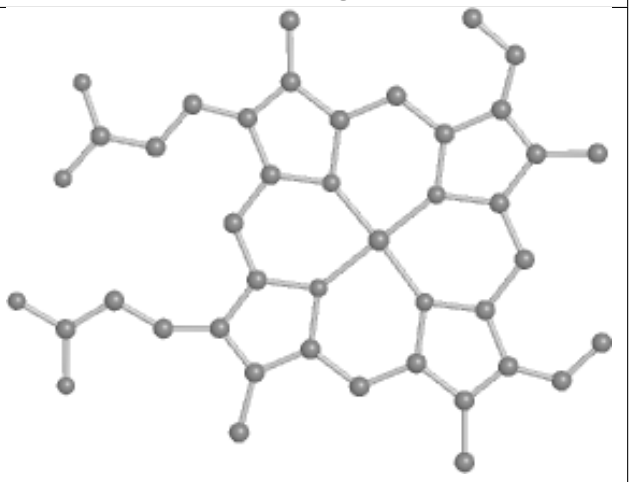
Bond lengths



Bond angles

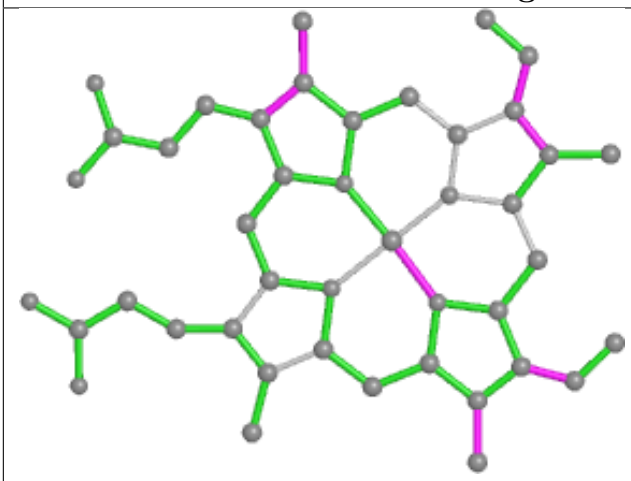


Torsions

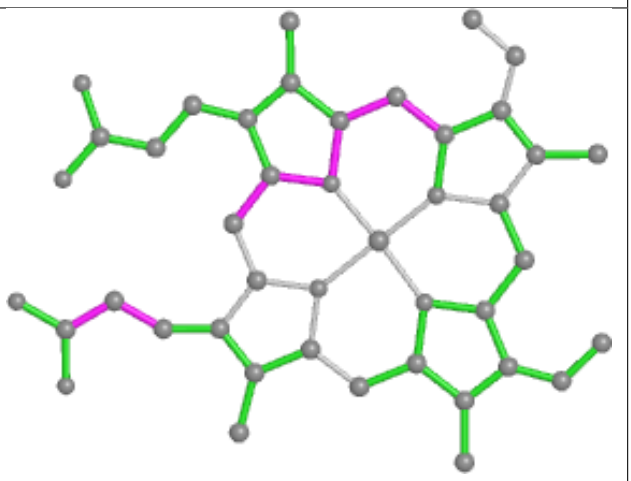


Rings

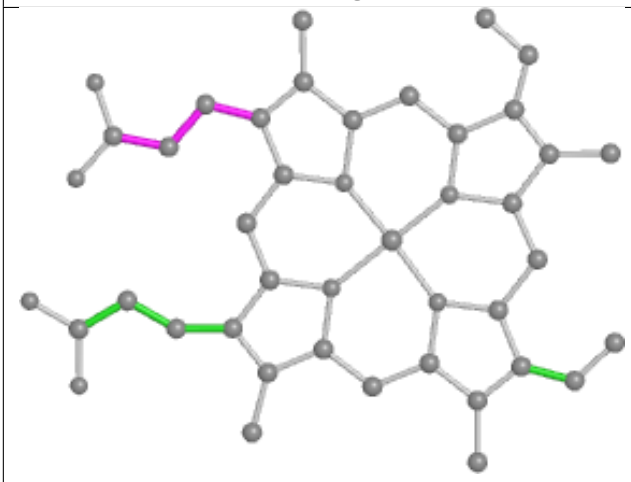
Ligand HEM V 201



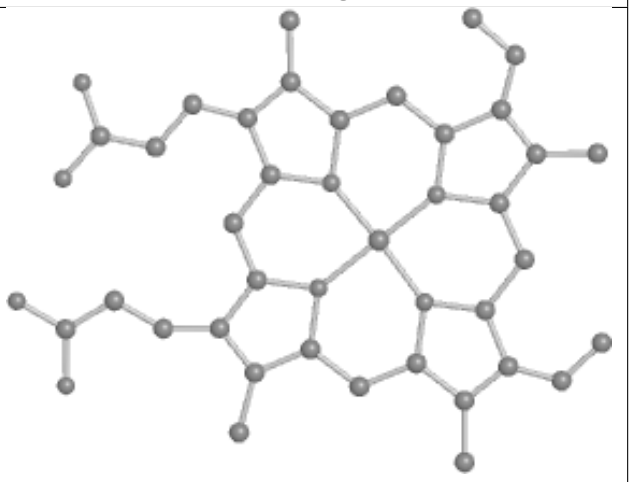
Bond lengths



Bond angles

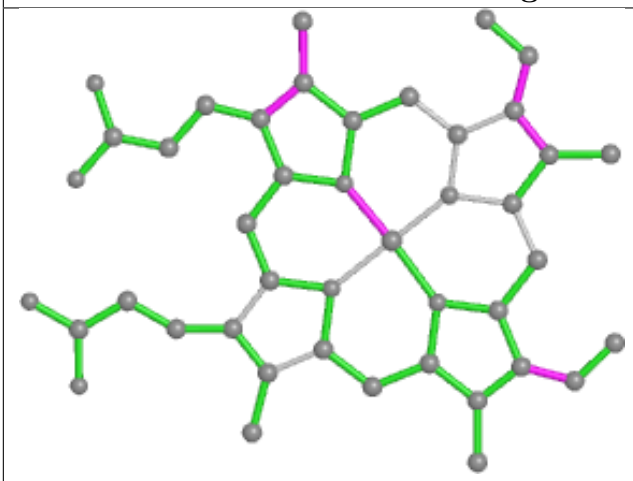


Torsions

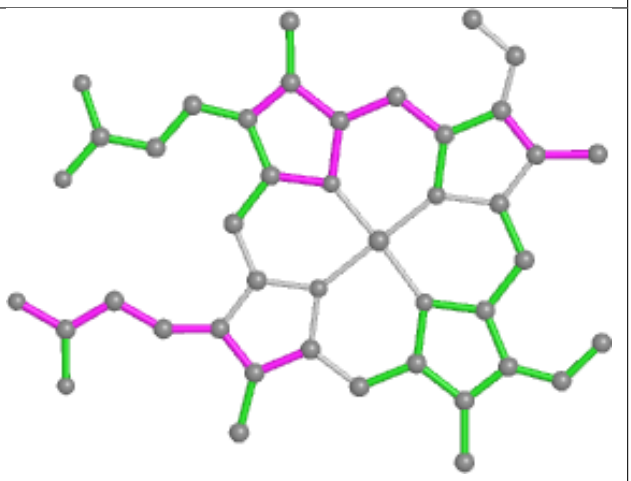


Rings

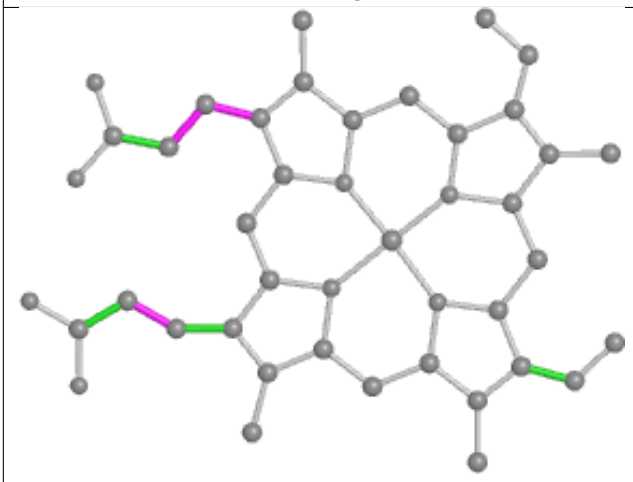
Ligand HEM Z 201



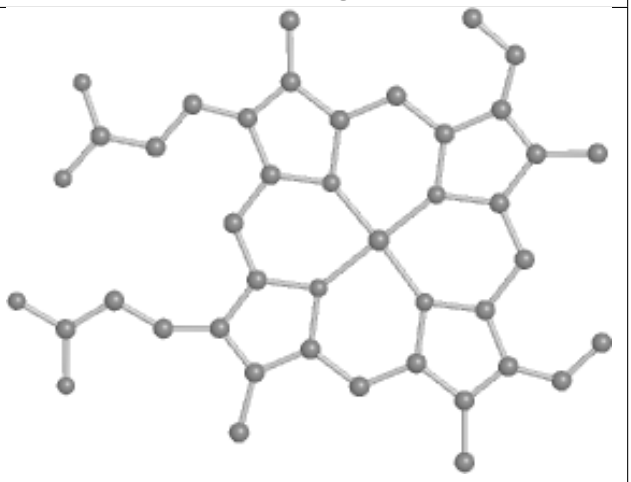
Bond lengths



Bond angles

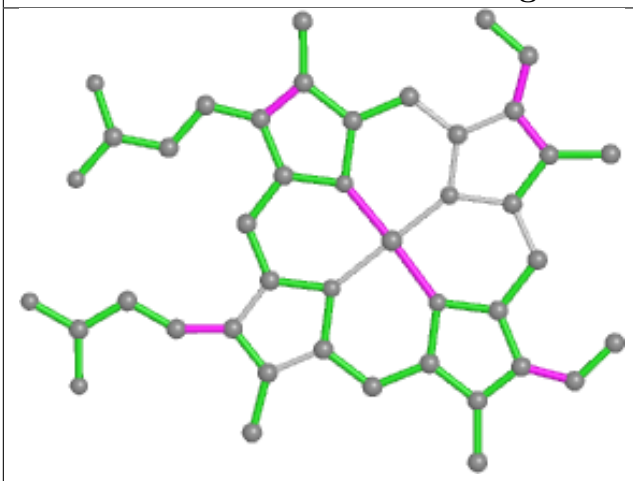


Torsions

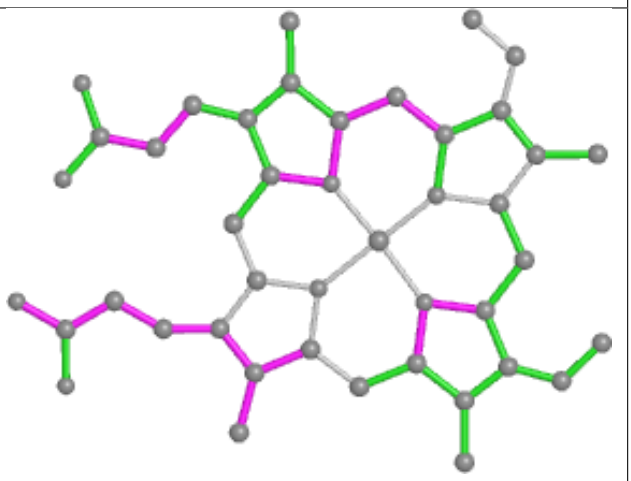


Rings

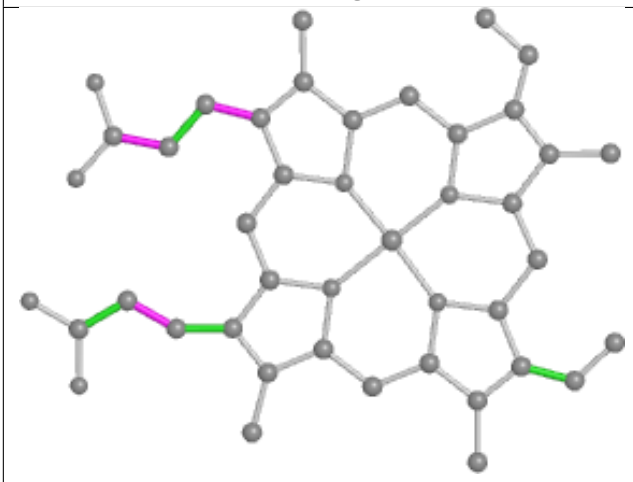
Ligand HEM P 201



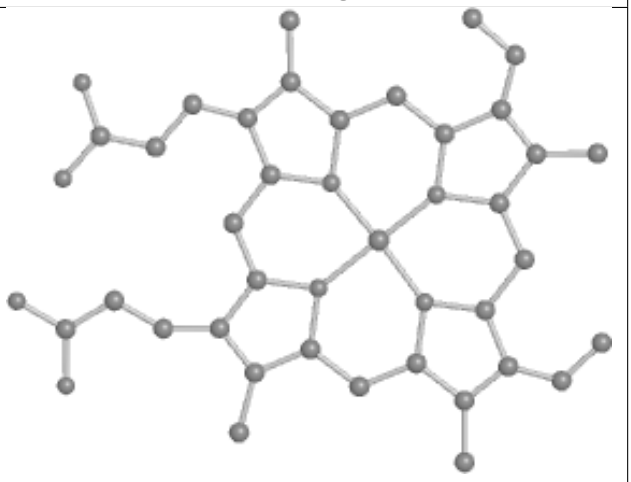
Bond lengths



Bond angles

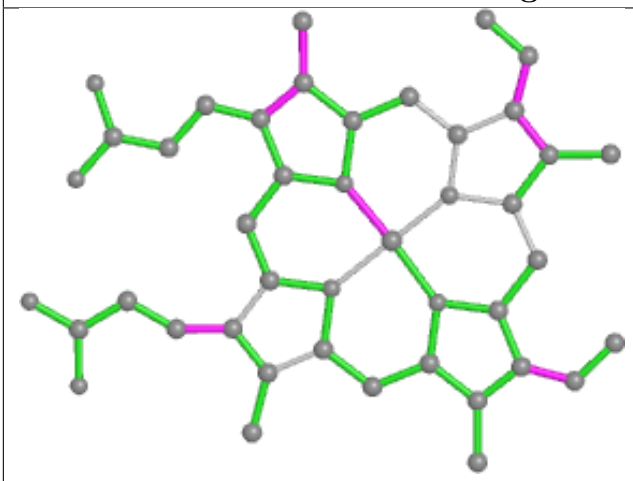


Torsions

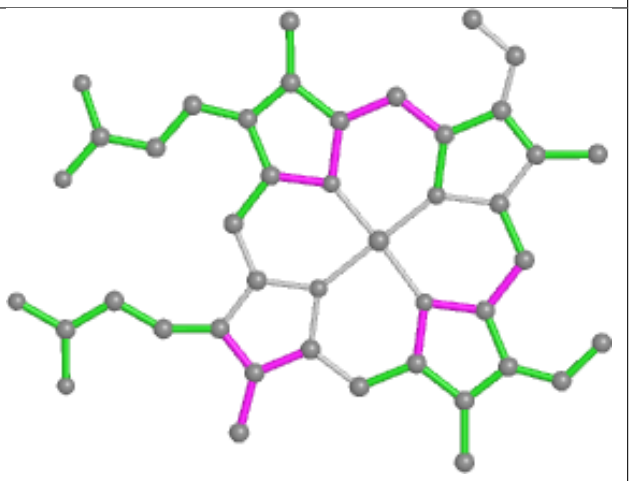


Rings

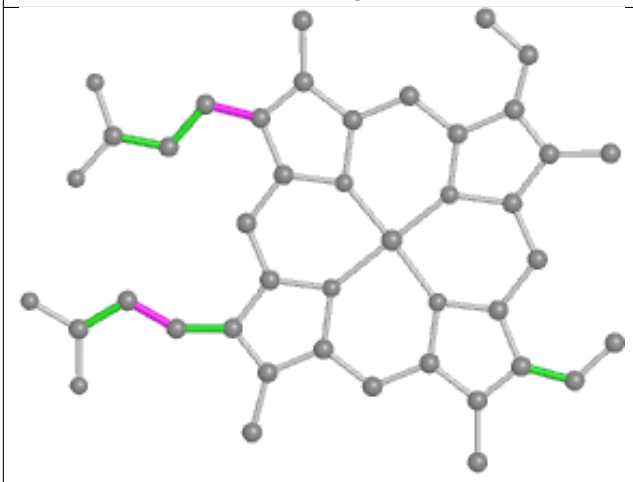
Ligand HEM F 201



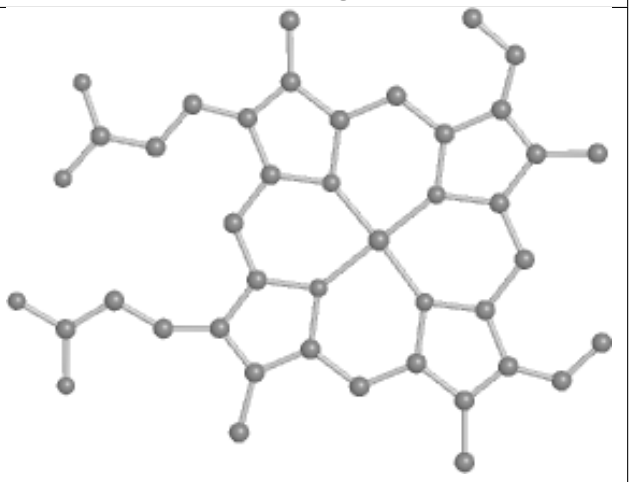
Bond lengths



Bond angles

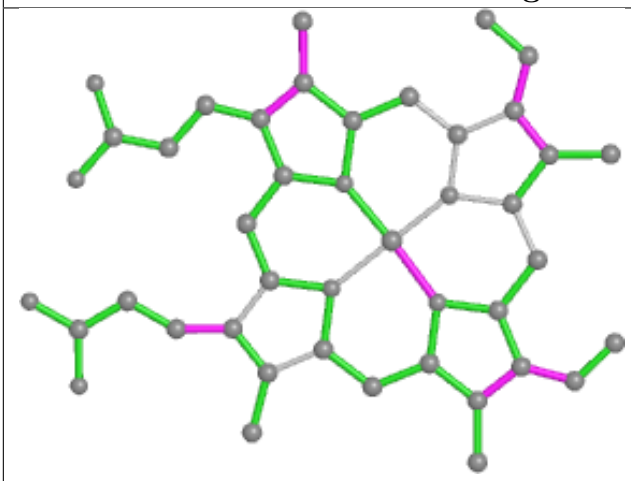


Torsions

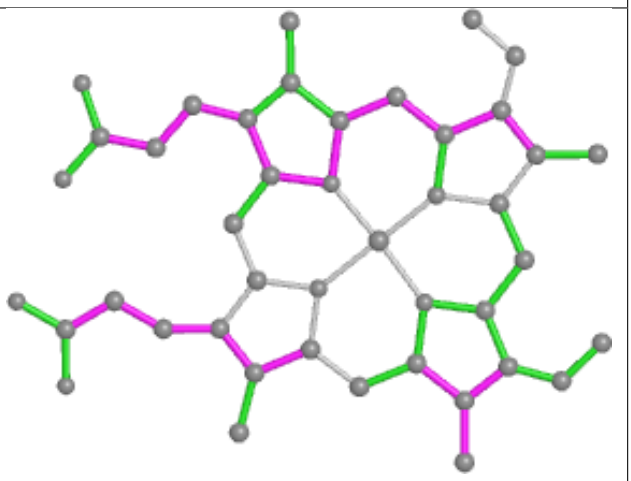


Rings

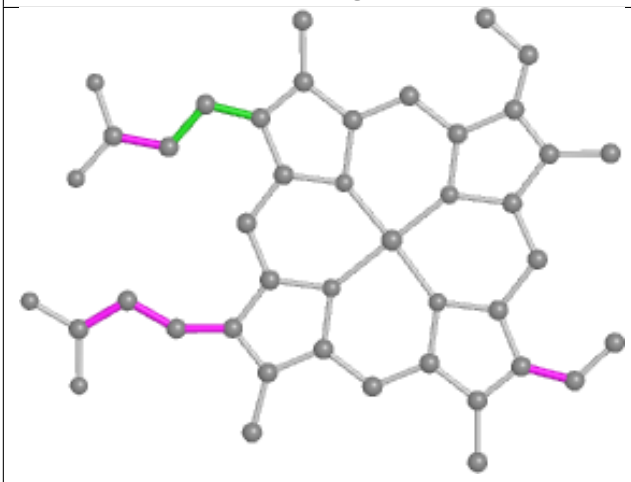
Ligand HEM 1 201



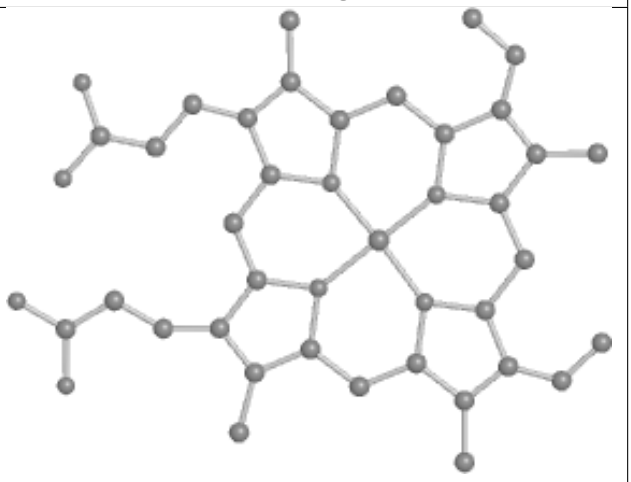
Bond lengths



Bond angles

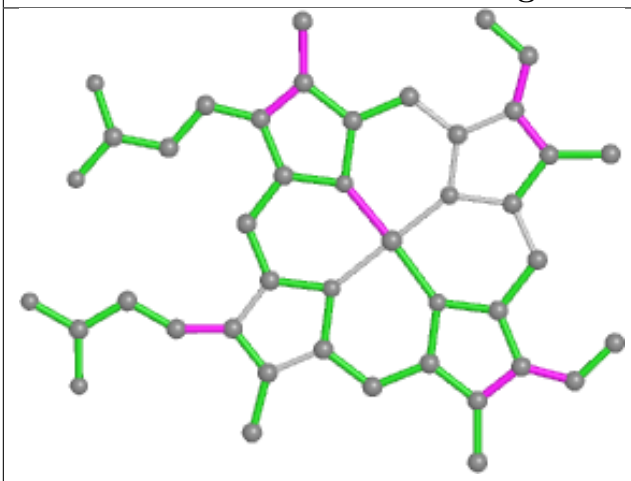


Torsions

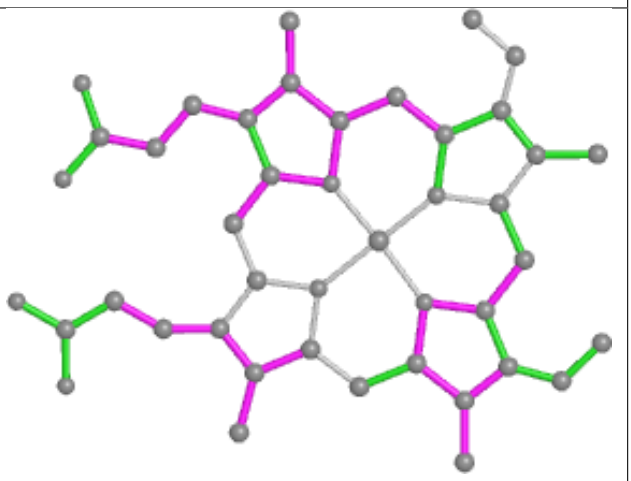


Rings

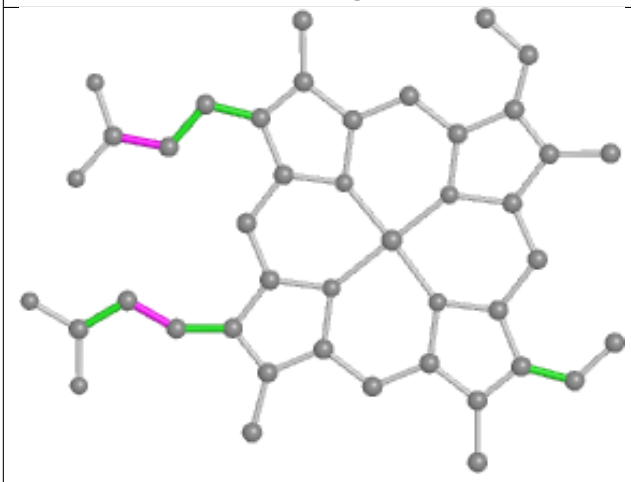
Ligand HEM K 201



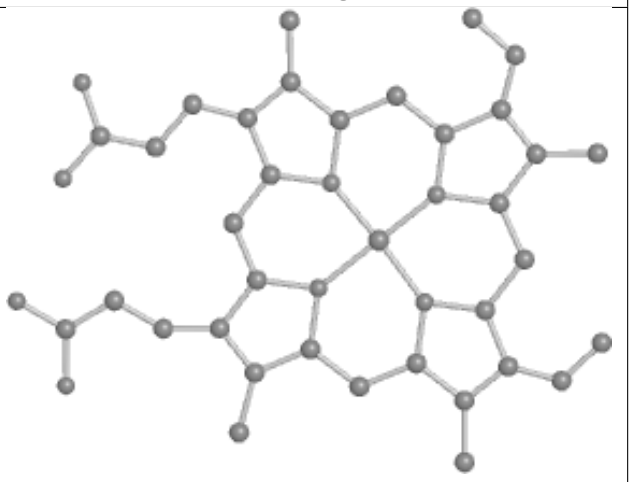
Bond lengths



Bond angles

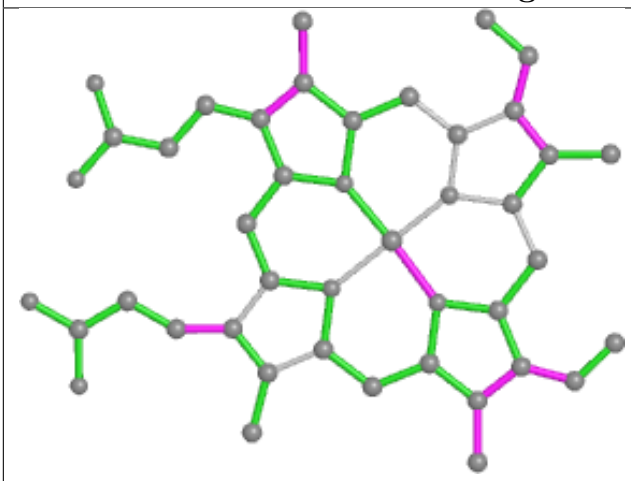


Torsions

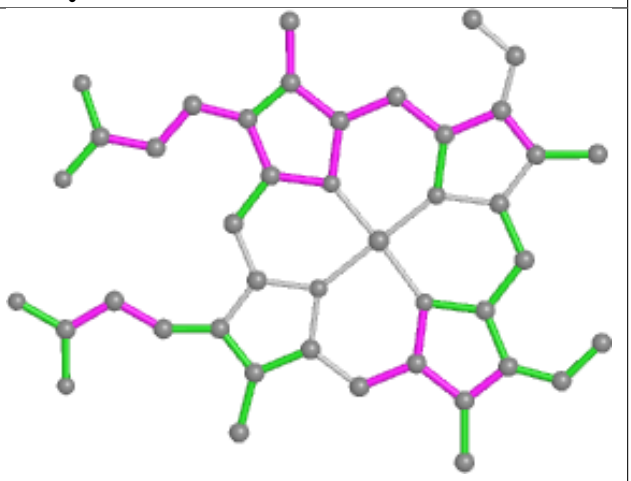


Rings

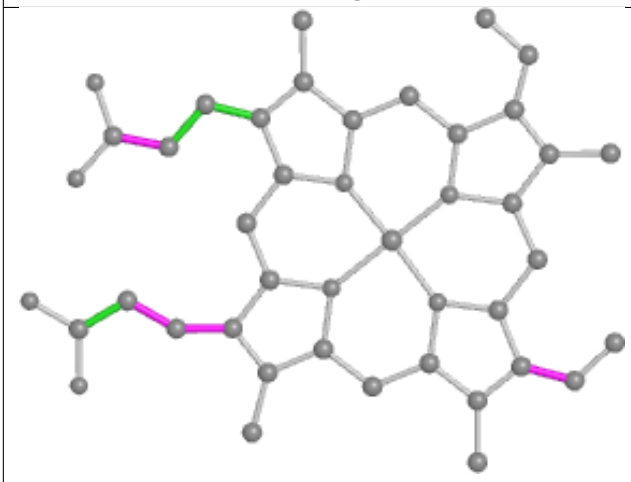
Ligand HEM Q 201



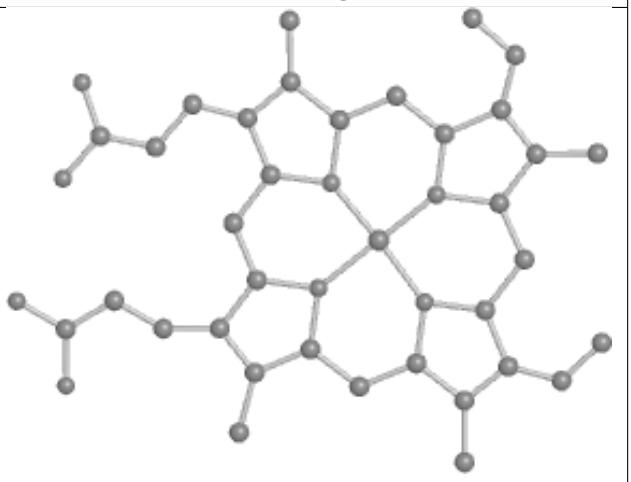
Bond lengths



Bond angles

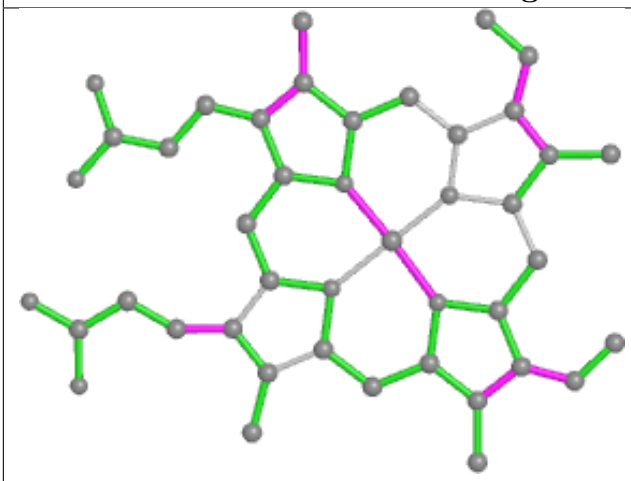


Torsions

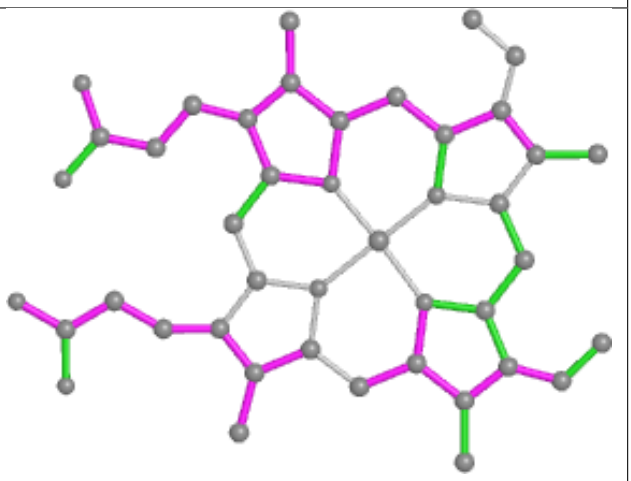


Rings

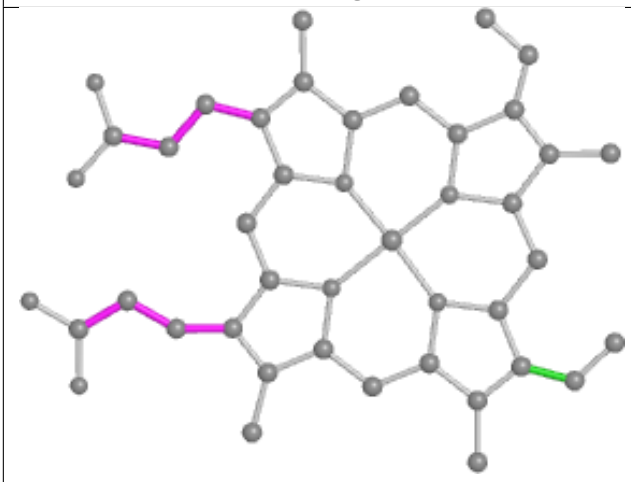
Ligand HEM L 201



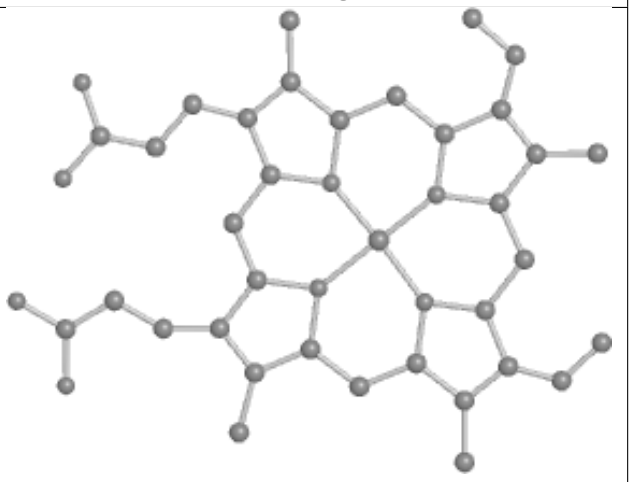
Bond lengths



Bond angles

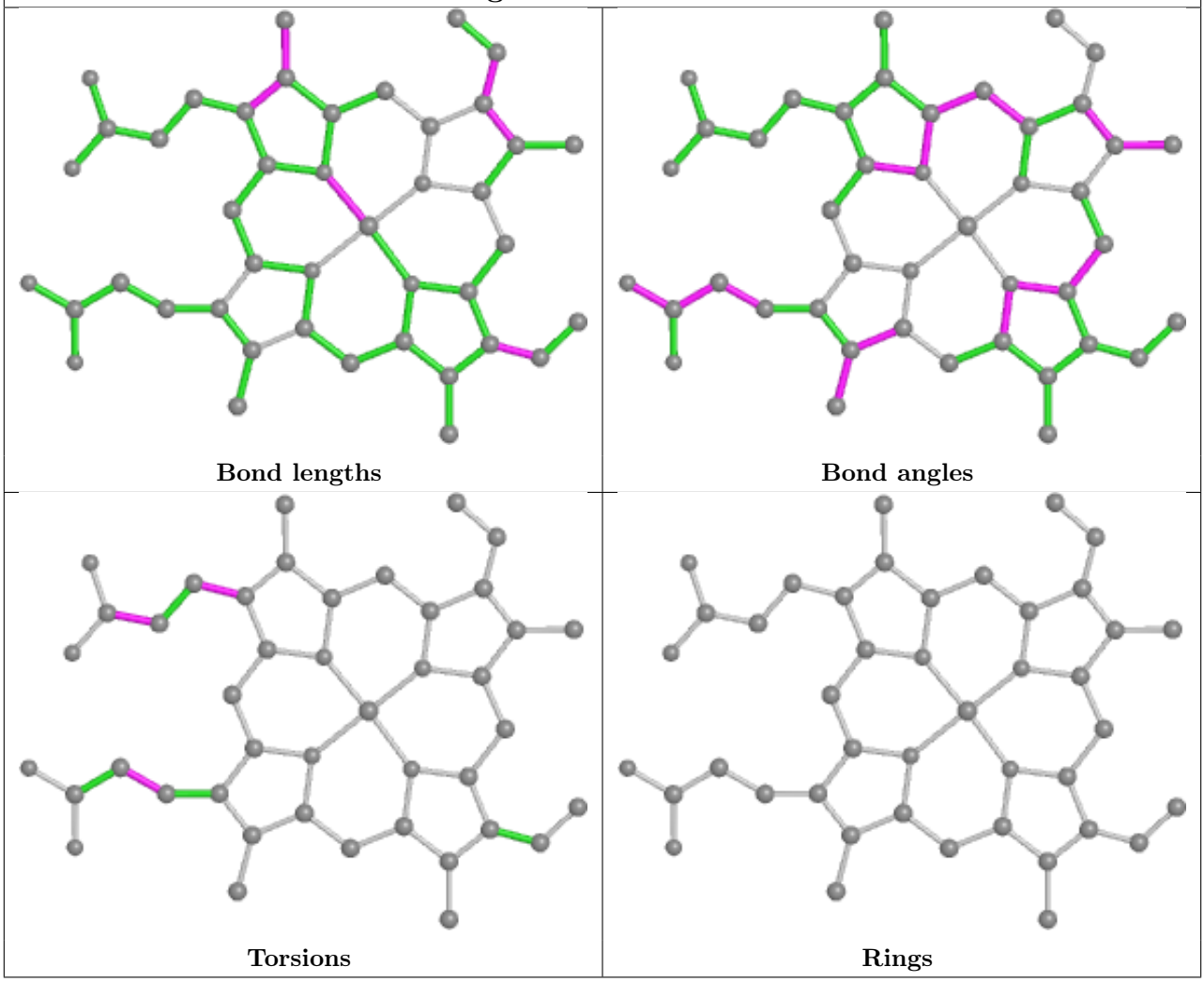


Torsions



Rings

Ligand HEM A 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	141/141 (100%)	-0.38	0	100	100	40, 52, 72, 81	0
1	F	141/141 (100%)	-0.37	0	100	100	49, 67, 83, 92	0
1	K	141/141 (100%)	-0.39	0	100	100	37, 53, 76, 86	0
1	P	141/141 (100%)	-0.41	0	100	100	53, 67, 91, 107	0
1	U	141/141 (100%)	-0.30	0	100	100	59, 76, 98, 100	0
1	Z	141/141 (100%)	-0.38	0	100	100	58, 72, 89, 93	0
2	1	146/146 (100%)	-0.41	1 (0%)	87	75	67, 79, 104, 138	0
2	B	146/146 (100%)	-0.37	0	100	100	39, 60, 90, 117	0
2	G	146/146 (100%)	-0.32	2 (1%)	75	56	50, 66, 97, 118	0
2	L	146/146 (100%)	-0.38	0	100	100	39, 62, 94, 120	0
2	Q	146/146 (100%)	-0.34	0	100	100	53, 69, 102, 133	0
2	V	146/146 (100%)	-0.36	0	100	100	66, 78, 105, 137	0
3	2	310/315 (98%)	-0.20	1 (0%)	94	88	63, 80, 96, 115	0
3	C	310/315 (98%)	-0.27	1 (0%)	94	88	38, 57, 75, 93	0
3	H	310/315 (98%)	-0.19	2 (0%)	89	78	56, 74, 94, 114	0
3	M	310/315 (98%)	-0.24	1 (0%)	94	88	38, 55, 79, 96	0
3	R	310/315 (98%)	-0.21	1 (0%)	94	88	65, 79, 100, 107	0
3	W	310/315 (98%)	-0.08	2 (0%)	89	78	76, 92, 112, 121	0
4	3	144/146 (98%)	-0.34	2 (1%)	75	56	60, 75, 95, 115	0
4	D	144/146 (98%)	-0.38	2 (1%)	75	56	51, 65, 84, 101	0
4	I	144/146 (98%)	-0.34	0	100	100	49, 72, 95, 111	0
4	N	144/146 (98%)	-0.30	2 (1%)	75	56	54, 68, 88, 100	0
4	S	144/146 (98%)	-0.34	0	100	100	53, 74, 94, 109	0
4	X	144/146 (98%)	-0.35	1 (0%)	87	75	61, 78, 100, 115	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
5	4	261/343 (76%)	-0.03	17 (6%)	18	8	74, 102, 153, 172	2 (0%)
5	E	261/343 (76%)	-0.06	13 (4%)	28	13	42, 82, 146, 155	2 (0%)
5	J	261/343 (76%)	0.23	23 (8%)	10	4	68, 110, 203, 212	2 (0%)
5	O	261/343 (76%)	-0.09	13 (4%)	28	13	43, 83, 140, 151	2 (0%)
5	T	261/343 (76%)	0.22	23 (8%)	10	4	68, 111, 197, 212	2 (0%)
5	Y	261/343 (76%)	0.26	25 (9%)	8	2	82, 111, 205, 213	2 (0%)
All	All	6012/6546 (91%)	-0.19	132 (2%)	62	41	37, 76, 138, 213	12 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	T	293	ALA	8.7
5	T	294	GLN	8.0
5	J	118	ALA	7.5
5	J	296	GLU	7.5
5	J	219	ASN	7.4
5	T	219	ASN	7.2
5	Y	294	GLN	7.1
5	Y	293	ALA	6.8
5	T	296	GLU	6.4
5	E	219	ASN	6.1
5	Y	296	GLU	6.1
5	T	118	ALA	6.0
5	Y	118	ALA	6.0
5	T	115	ASP	5.5
5	J	293	ALA	5.5
5	4	294	GLN	5.0
5	J	294	GLN	5.0
5	J	115	ASP	4.9
5	4	114	ASN	4.9
5	T	38	GLY	4.8
5	J	289	HIS	4.8
5	T	106	ARG	4.7
5	O	219	ASN	4.7
5	Y	291	THR	4.5
5	T	291	THR	4.5
5	J	290	GLU	4.4
5	Y	117	LYS	4.4
5	Y	290	GLU	4.4
4	3	228	SER	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	Y	114	ASN	4.1
5	Y	115	ASP	4.1
5	Y	219	ASN	4.1
5	Y	295	GLU	4.0
5	Y	289	HIS	4.0
5	4	185	ASN	3.9
5	4	291	THR	3.9
5	E	112	LYS	3.9
5	T	185	ASN	3.9
5	E	114	ASN	3.8
5	J	195	GLU	3.7
5	4	219	ASN	3.7
5	E	294	GLN	3.7
5	O	114	ASN	3.6
4	X	229	LEU	3.5
5	Y	185	ASN	3.5
5	J	114	ASN	3.4
5	J	106	ARG	3.4
5	T	295	GLU	3.4
5	Y	105	GLN	3.3
5	J	291	THR	3.3
5	J	185	ASN	3.3
5	Y	106	ARG	3.3
5	J	295	GLU	3.3
5	T	114	ASN	3.3
5	4	189	ASP	3.3
5	4	220	VAL	3.2
5	T	111	GLY	3.2
5	O	185	ASN	3.2
5	J	38	GLY	3.2
5	4	195	GLU	3.1
4	D	229	LEU	3.1
5	4	112	LYS	3.1
5	T	195	GLU	3.1
5	O	294	GLN	3.1
5	T	290	GLU	3.1
5	O	291	THR	3.1
5	Y	109	GLU	3.0
3	2	93	PRO	3.0
5	T	105	GLN	3.0
5	Y	189	ASP	3.0
5	Y	38	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	93	PRO	2.9
5	Y	191	LYS	2.9
4	N	228	SER	2.9
4	N	229	LEU	2.8
5	J	105	GLN	2.8
5	O	184	GLY	2.8
5	E	38	GLY	2.8
5	4	183	LYS	2.8
3	C	93	PRO	2.8
5	Y	110	LEU	2.8
5	J	117	LYS	2.8
3	W	353	SER	2.7
5	O	38	GLY	2.7
5	T	289	HIS	2.7
5	Y	113	ALA	2.6
5	E	290	GLU	2.6
5	E	191	LYS	2.6
2	G	146	HIS	2.6
5	E	227	LYS	2.5
5	E	185	ASN	2.5
5	O	284	GLU	2.5
5	E	184	GLY	2.4
5	T	286	LYS	2.4
5	4	116	THR	2.4
5	J	36	ALA	2.4
3	H	157	ASN	2.4
5	E	41	THR	2.4
5	O	183	LYS	2.4
5	Y	36	ALA	2.3
5	E	183	LYS	2.3
4	3	229	LEU	2.3
3	M	93	PRO	2.3
5	J	186	GLY	2.3
5	T	112	LYS	2.3
5	O	290	GLU	2.3
4	D	178	VAL	2.3
5	T	191	LYS	2.3
2	1	2	HIS	2.3
5	Y	269	LYS	2.2
5	E	284	GLU	2.2
3	R	93	PRO	2.2
5	Y	286	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	T	186	GLY	2.2
5	J	286	LYS	2.2
5	O	196	LYS	2.2
3	W	93	PRO	2.2
5	O	41	THR	2.2
5	J	111	GLY	2.2
5	T	183	LYS	2.2
5	4	186	GLY	2.2
5	4	184	GLY	2.1
5	J	183	LYS	2.1
5	J	41	THR	2.1
5	O	191	LYS	2.1
5	Y	217	ALA	2.1
5	4	290	GLU	2.1
5	4	38	GLY	2.1
5	T	117	LYS	2.1
5	4	191	LYS	2.1
5	4	36	ALA	2.0
2	G	2	HIS	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	f	1	14/15	0.69	0.33	105,105,105,105	0
6	NAG	i	1	14/15	0.70	0.37	118,118,118,118	0
6	NAG	d	1	14/15	0.71	0.32	90,90,90,90	0
6	NAG	h	2	14/15	0.74	0.23	116,116,116,116	0
6	NAG	g	2	14/15	0.78	0.22	94,94,94,94	0
6	NAG	a	1	14/15	0.78	0.30	86,86,86,86	0
6	NAG	c	2	14/15	0.78	0.22	98,98,98,98	0
6	NAG	d	2	14/15	0.80	0.40	97,97,97,97	0
6	NAG	e	2	14/15	0.81	0.22	86,86,86,86	0

Continued on next page...

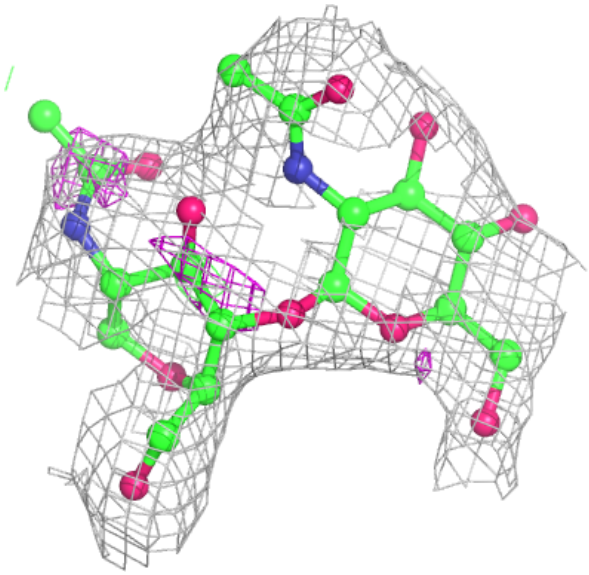
Continued from previous page...

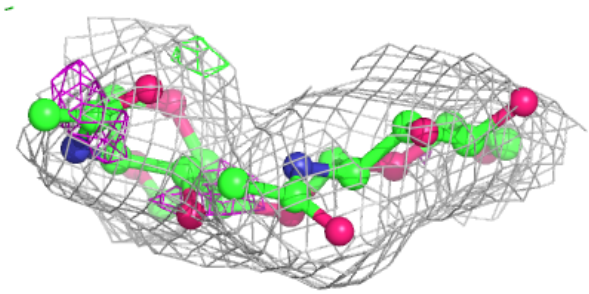
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	j	2	14/15	0.81	0.18	106,106,106,106	0
6	NAG	i	2	14/15	0.82	0.36	123,123,123,123	0
6	NAG	b	2	14/15	0.82	0.17	89,89,89,89	0
6	NAG	f	2	14/15	0.83	0.38	112,112,112,112	0
6	NAG	e	1	14/15	0.84	0.21	75,75,75,75	0
6	NAG	c	1	14/15	0.85	0.23	89,89,89,89	0
6	NAG	h	1	14/15	0.85	0.22	107,107,107,107	0
6	NAG	b	1	14/15	0.87	0.18	77,77,77,77	0
6	NAG	g	1	14/15	0.87	0.20	88,88,88,88	0
6	NAG	j	1	14/15	0.89	0.22	97,97,97,97	0
6	NAG	a	2	14/15	0.90	0.31	94,94,94,94	0

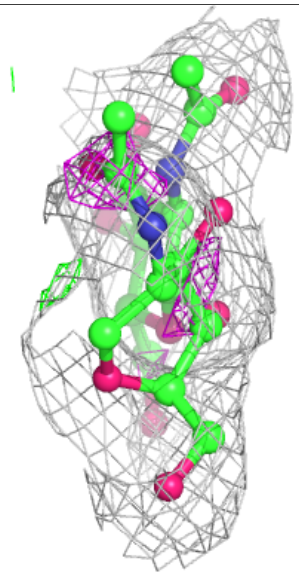
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain a:

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

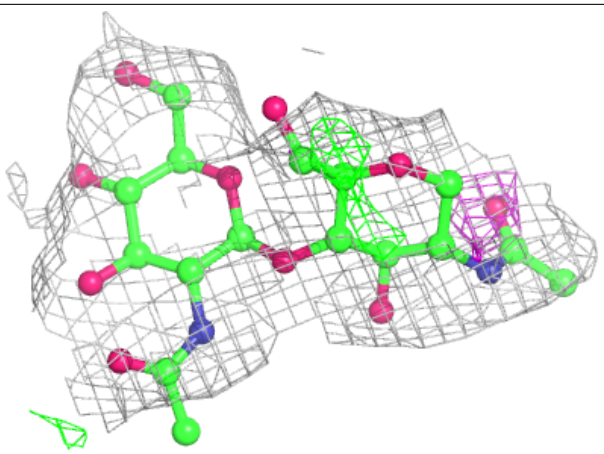


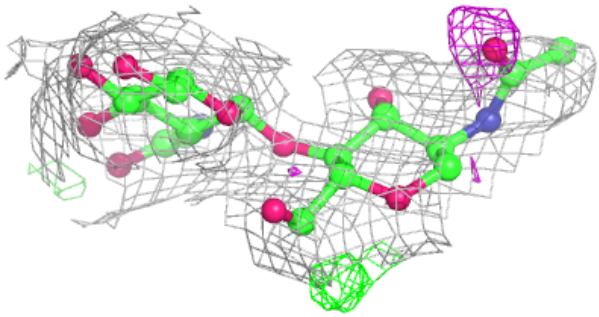


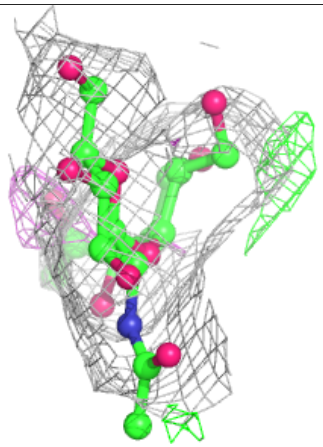


Electron density around Chain b:

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

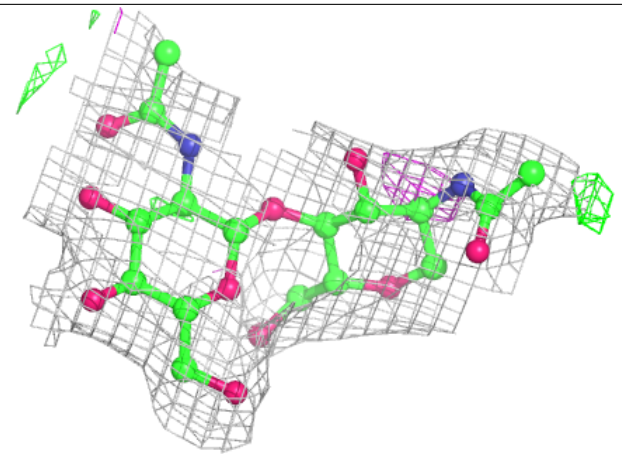


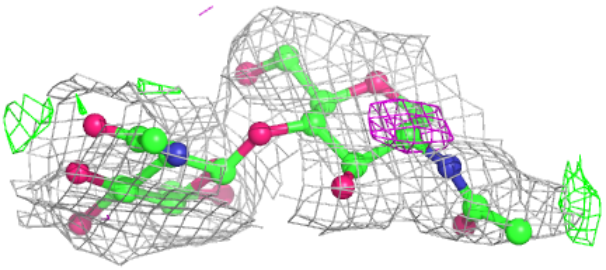


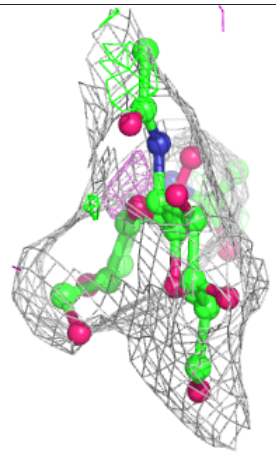


Electron density around Chain c:

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

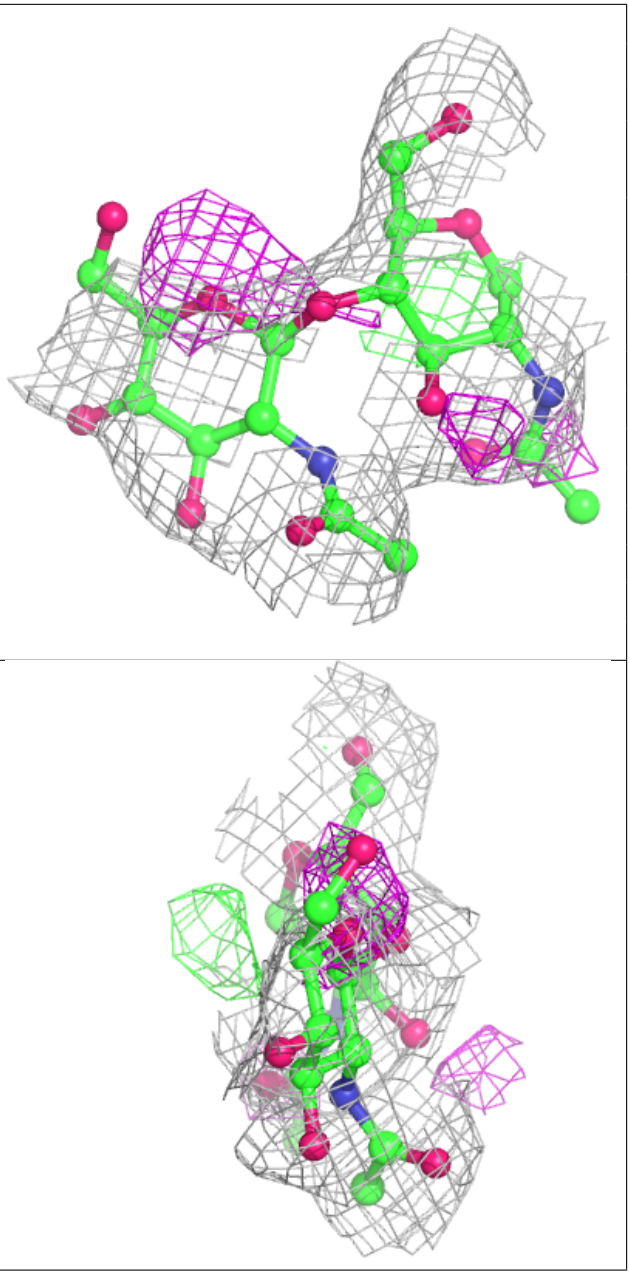






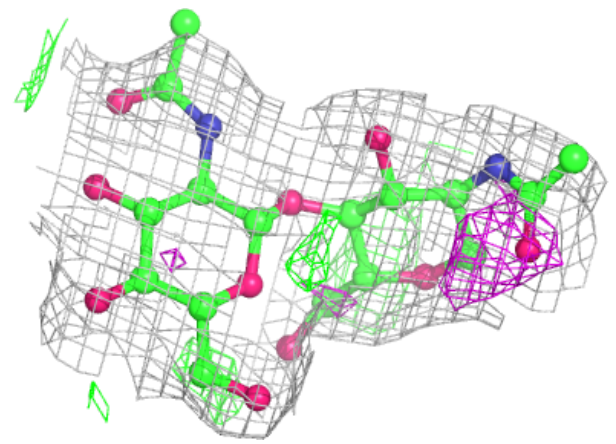
Electron density around Chain d:

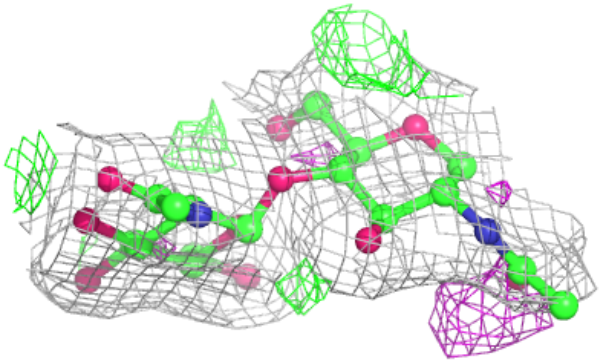
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

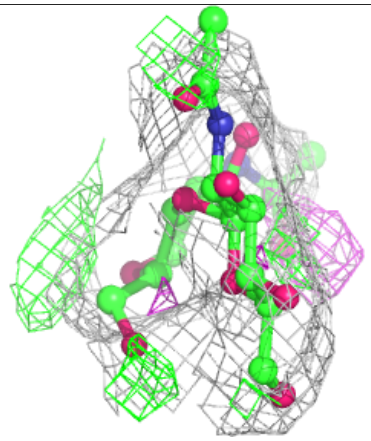


Electron density around Chain e:

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

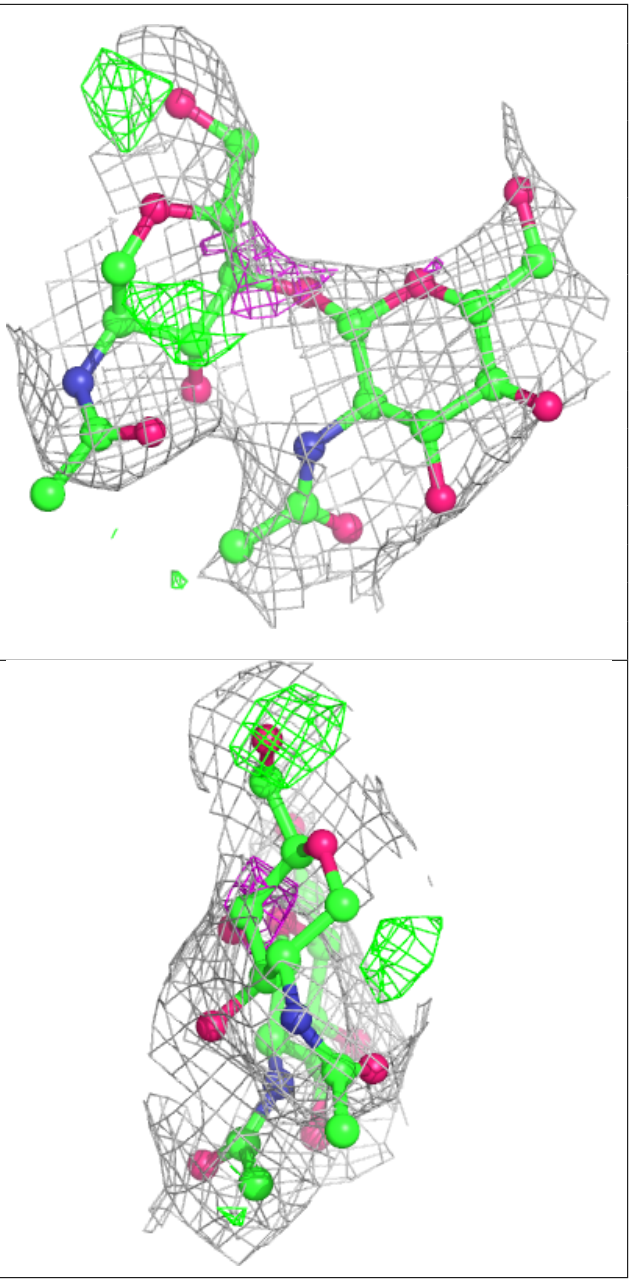






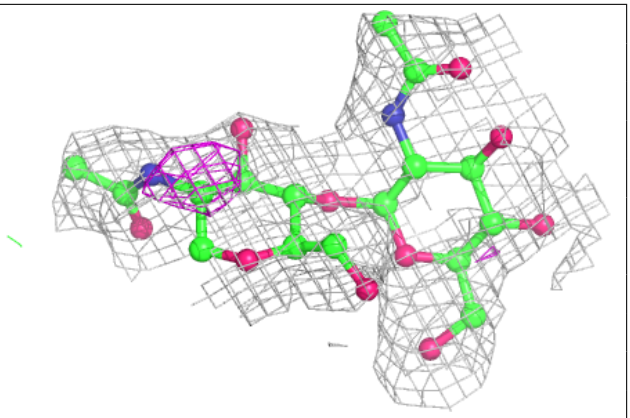
Electron density around Chain f:

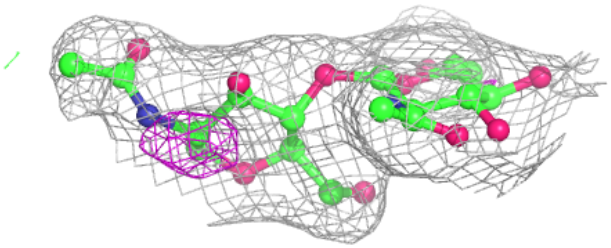
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

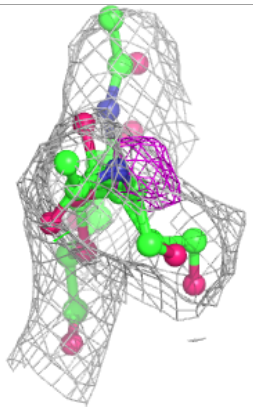


Electron density around Chain g:

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

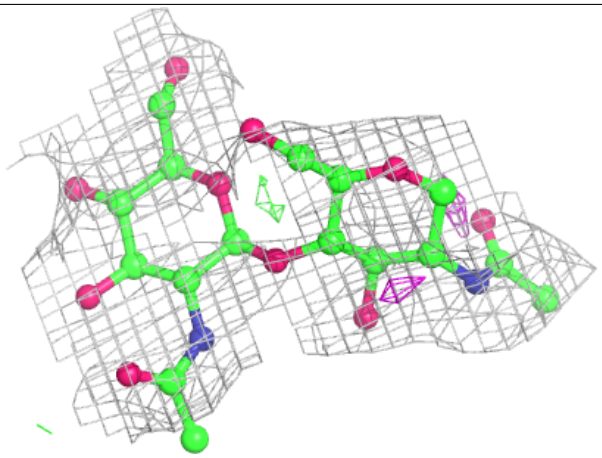


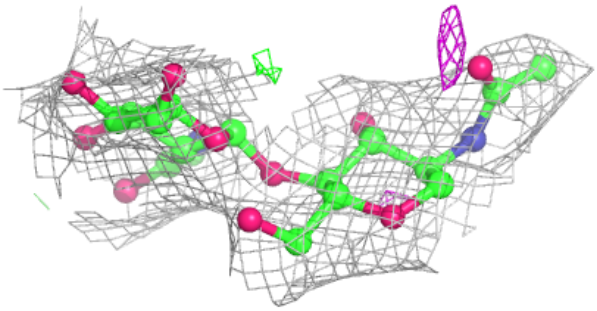


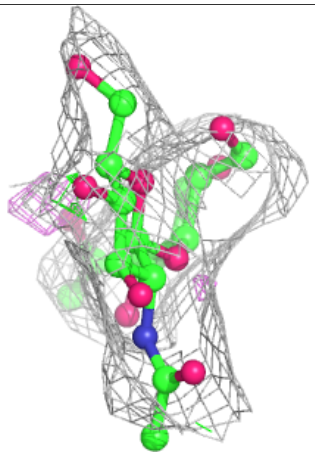


Electron density around Chain h:

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

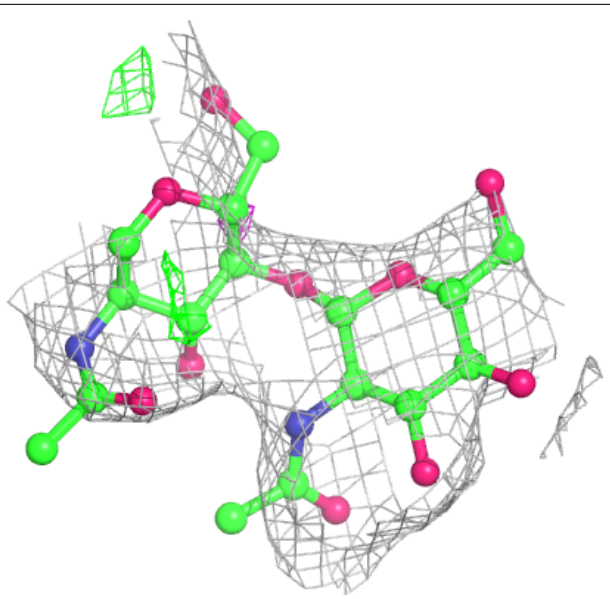


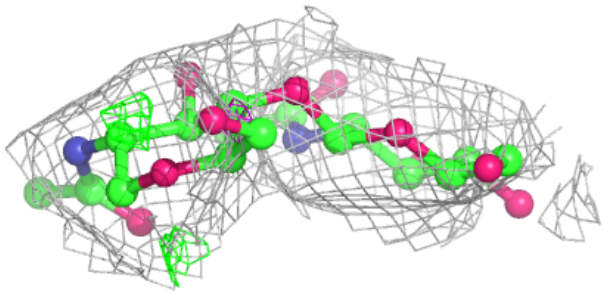


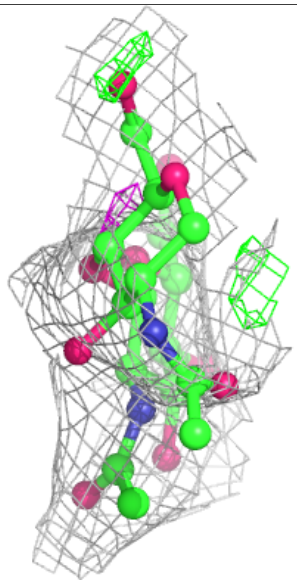


Electron density around Chain i:

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

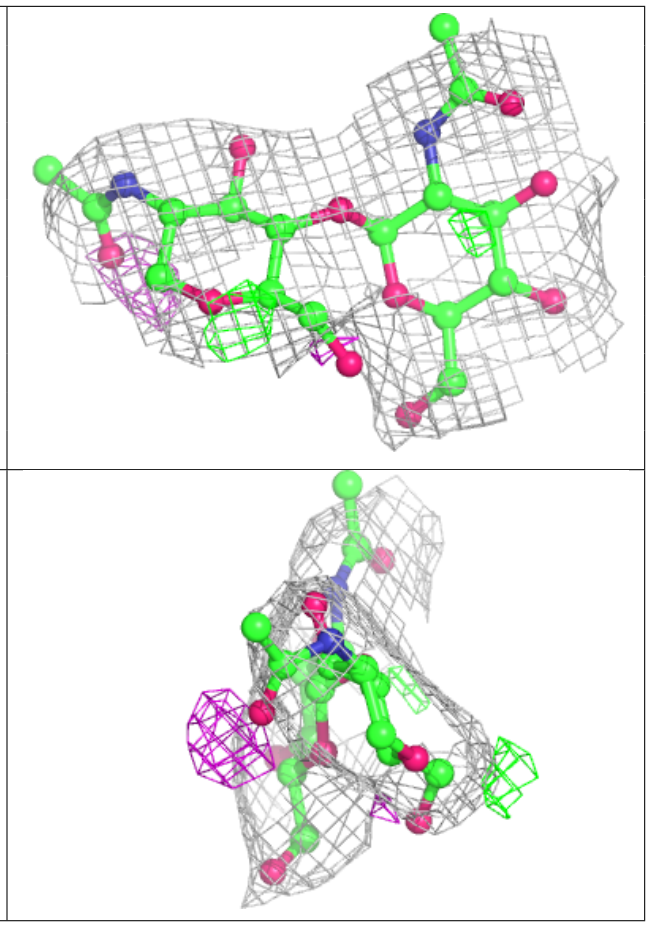






Electron density around Chain j:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	R	1004	14/15	0.48	0.50	123,123,123,123	0
9	NAG	W	1002	14/15	0.66	0.33	112,112,112,112	0
9	NAG	M	1004	14/15	0.69	0.44	116,116,116,116	0
9	NAG	C	1004	14/15	0.71	0.48	112,112,112,112	0
9	NAG	T	1001	14/15	0.73	0.50	143,148,153,154	0
9	NAG	J	1001	14/15	0.75	0.50	136,144,151,154	0
9	NAG	H	1002	14/15	0.76	0.26	85,85,85,85	0
9	NAG	C	1001	14/15	0.79	0.42	84,84,84,84	0
9	NAG	O	1001	14/15	0.80	0.39	101,107,112,116	0
9	NAG	4	1001	14/15	0.80	0.45	125,128,131,132	0
9	NAG	Y	1001	14/15	0.82	0.39	133,142,147,151	0
9	NAG	R	1001	14/15	0.83	0.39	94,94,94,94	0

Continued on next page...

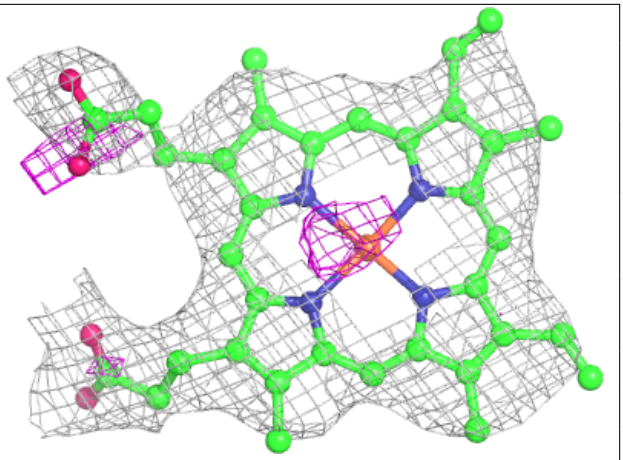
Continued from previous page...

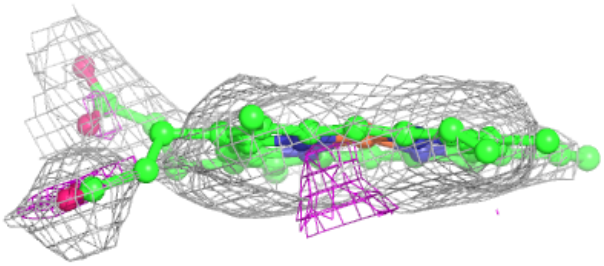
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	M	1001	14/15	0.83	0.40	92,92,92,92	0
9	NAG	Y	1002	14/15	0.84	0.22	81,85,88,90	0
9	NAG	2	1001	14/15	0.86	0.37	101,101,101,101	0
9	NAG	E	1001	14/15	0.86	0.42	103,107,112,113	0
9	NAG	W	1001	14/15	0.88	0.39	101,101,101,101	0
9	NAG	O	1002	14/15	0.88	0.17	60,65,68,70	0
9	NAG	J	1002	14/15	0.90	0.17	80,83,86,87	0
9	NAG	H	1001	14/15	0.90	0.36	81,81,81,81	0
9	NAG	4	1002	14/15	0.91	0.19	81,83,86,87	0
9	NAG	E	1002	14/15	0.92	0.14	63,67,70,70	0
9	NAG	T	1002	14/15	0.93	0.11	76,80,86,86	0
8	OXY	Q	202	2/2	0.93	0.31	62,62,62,63	0
7	HEM	F	201	43/43	0.94	0.23	56,65,76,80	0
8	OXY	A	202	2/2	0.94	0.31	61,61,61,62	0
7	HEM	Q	201	43/43	0.95	0.23	58,60,62,63	0
7	HEM	U	201	43/43	0.95	0.22	68,78,88,92	0
7	HEM	Z	201	43/43	0.95	0.21	63,71,79,82	0
7	HEM	1	201	43/43	0.95	0.24	63,68,73,76	0
7	HEM	A	201	43/43	0.95	0.21	51,55,60,62	0
7	HEM	G	201	43/43	0.95	0.23	53,58,64,67	0
8	OXY	U	202	2/2	0.95	0.25	80,80,80,81	0
7	HEM	K	201	43/43	0.95	0.20	43,57,69,73	0
7	HEM	L	201	43/43	0.95	0.21	45,50,57,59	0
7	HEM	P	201	43/43	0.95	0.22	63,71,79,83	0
7	HEM	B	201	43/43	0.96	0.23	41,50,60,64	0
8	OXY	Z	202	2/2	0.96	0.19	75,75,75,76	0
8	OXY	G	202	2/2	0.96	0.28	59,59,59,60	0
8	OXY	K	202	2/2	0.96	0.24	62,62,62,64	0
7	HEM	V	201	43/43	0.96	0.21	65,69,74,76	0
8	OXY	B	202	2/2	0.97	0.22	49,49,49,51	0
8	OXY	F	202	2/2	0.97	0.29	72,72,72,72	0
8	OXY	L	202	2/2	0.98	0.19	47,47,47,47	0
8	OXY	P	202	2/2	0.98	0.23	70,70,70,72	0
8	OXY	V	202	2/2	0.98	0.17	69,69,69,69	0
8	OXY	1	202	2/2	0.99	0.21	69,69,69,69	0

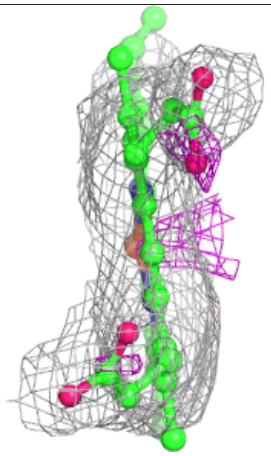
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM F 201:

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

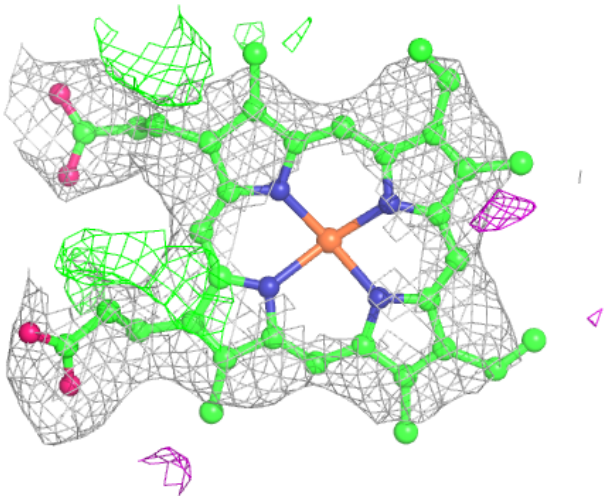


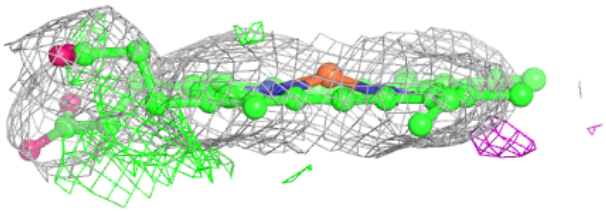


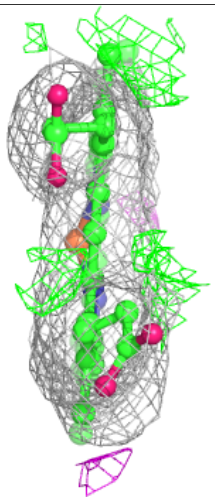


Electron density around HEM Q 201:

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

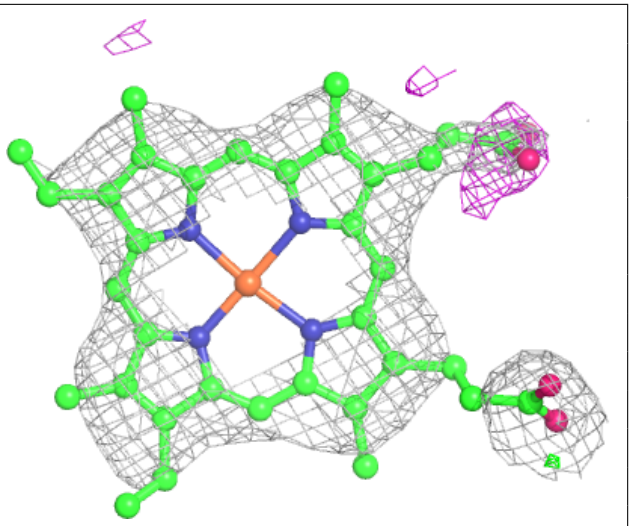


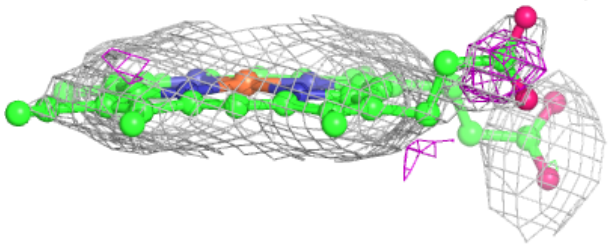


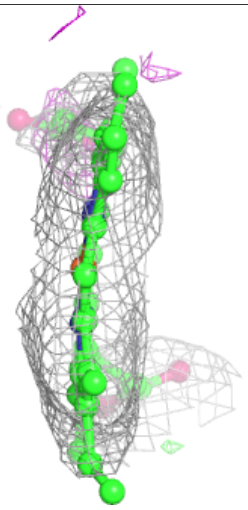


Electron density around HEM U 201:

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

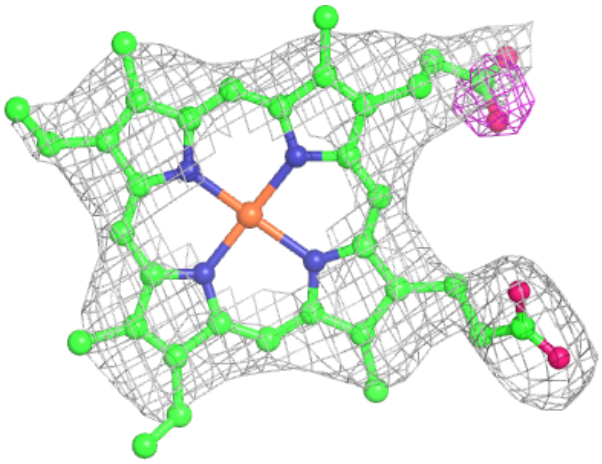


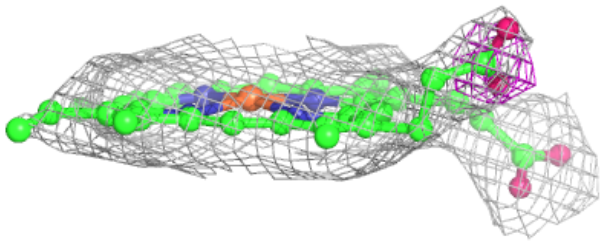


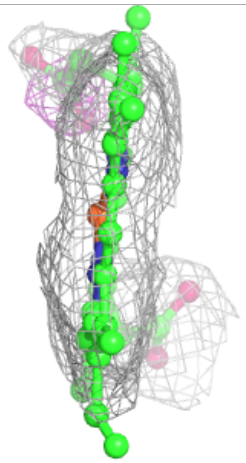


Electron density around HEM Z 201:

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

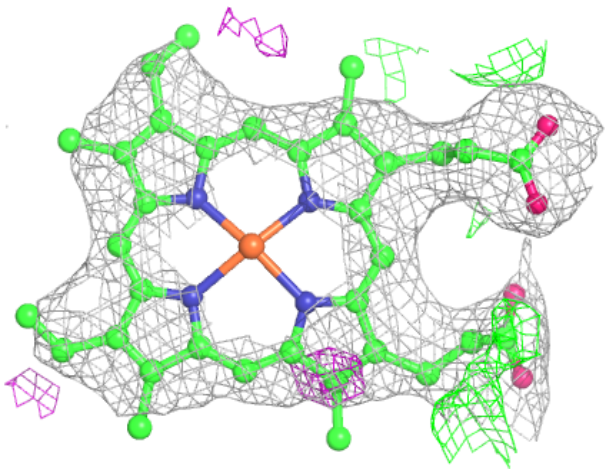


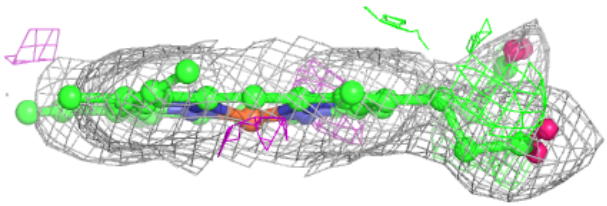


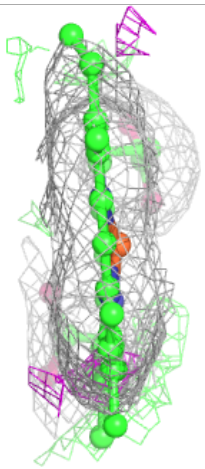


Electron density around HEM 1 201:

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

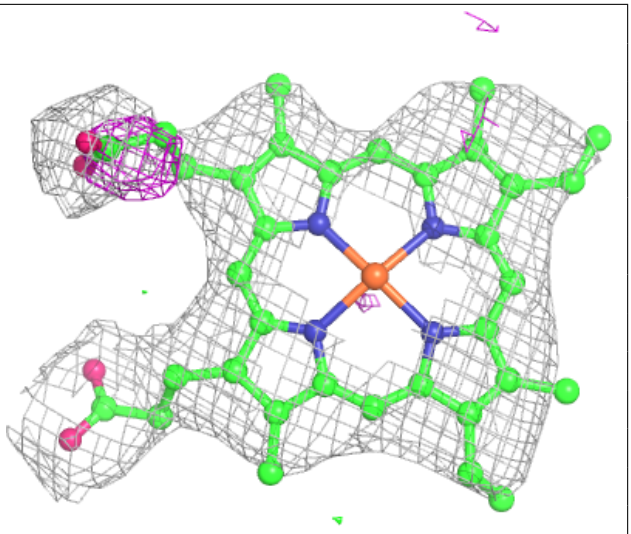


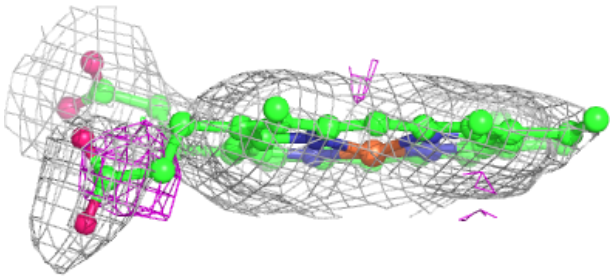


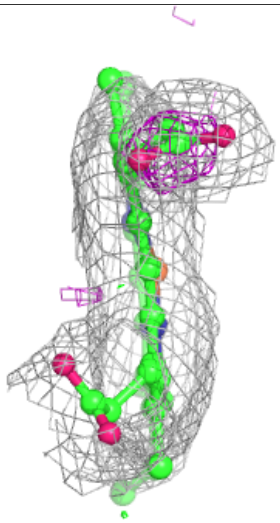


Electron density around HEM A 201:

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

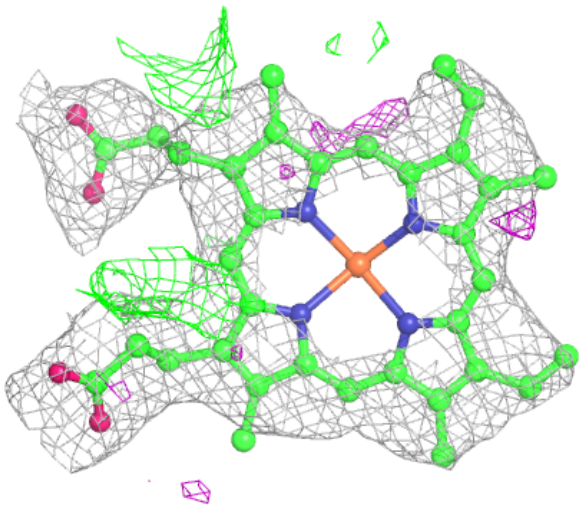


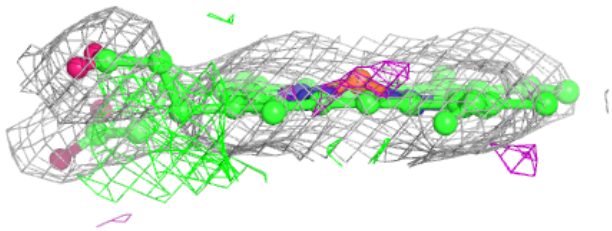




Electron density around HEM G 201:

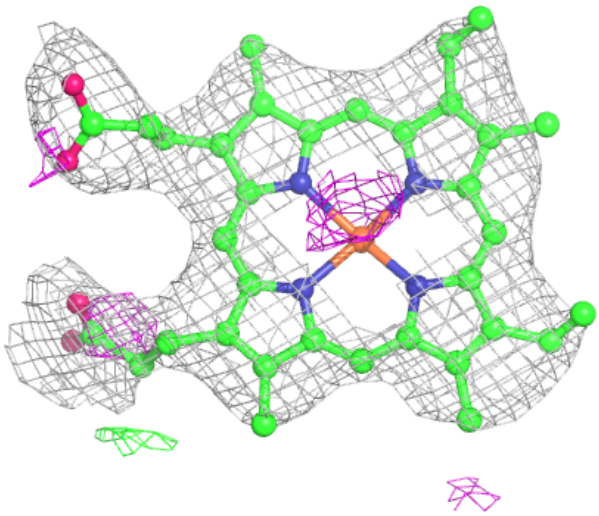
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

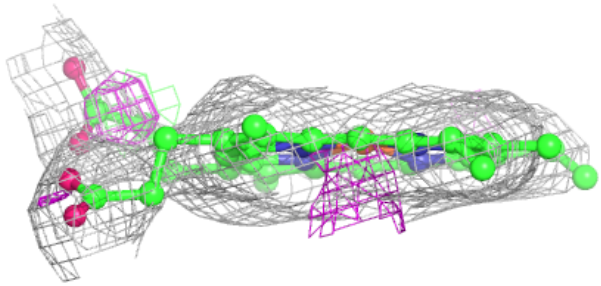




Electron density around HEM K 201:

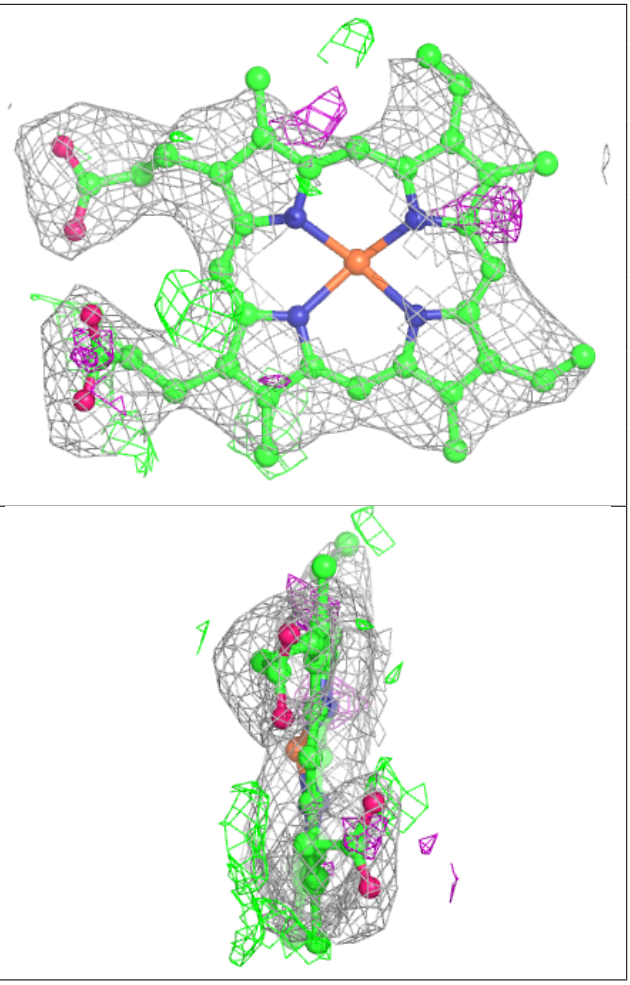
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





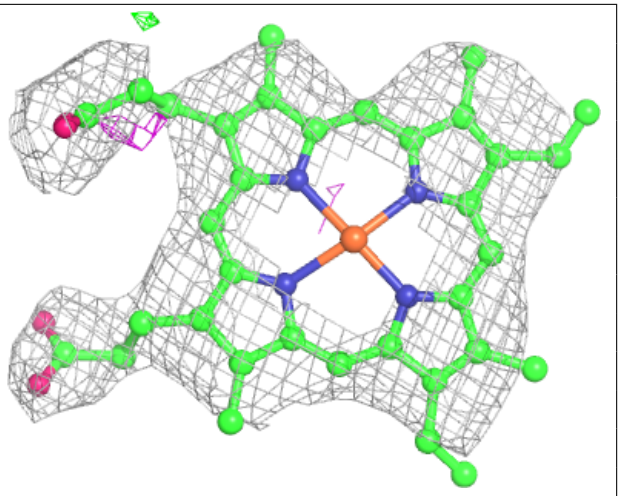
Electron density around HEM L 201:

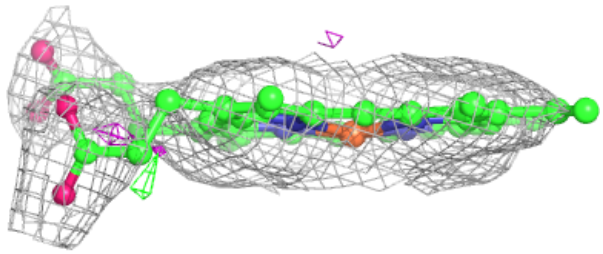
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

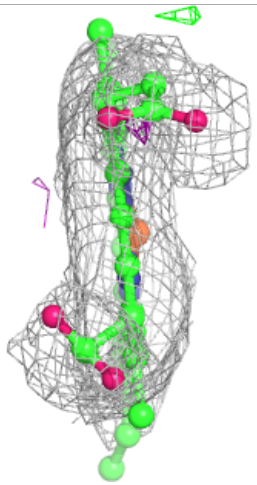


Electron density around HEM P 201:

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

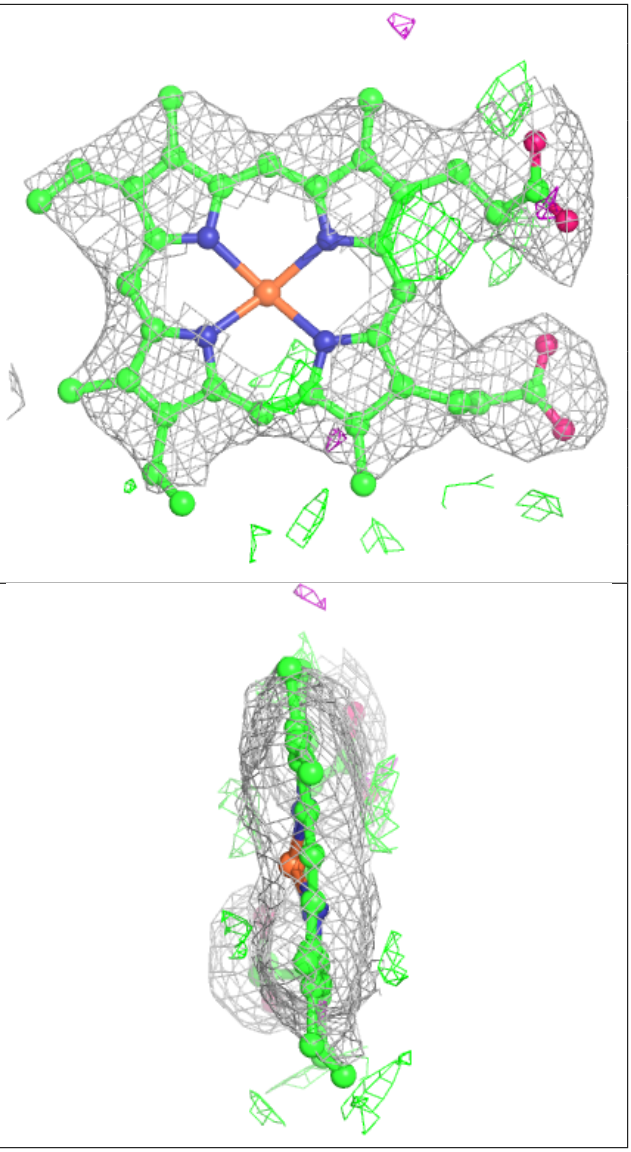






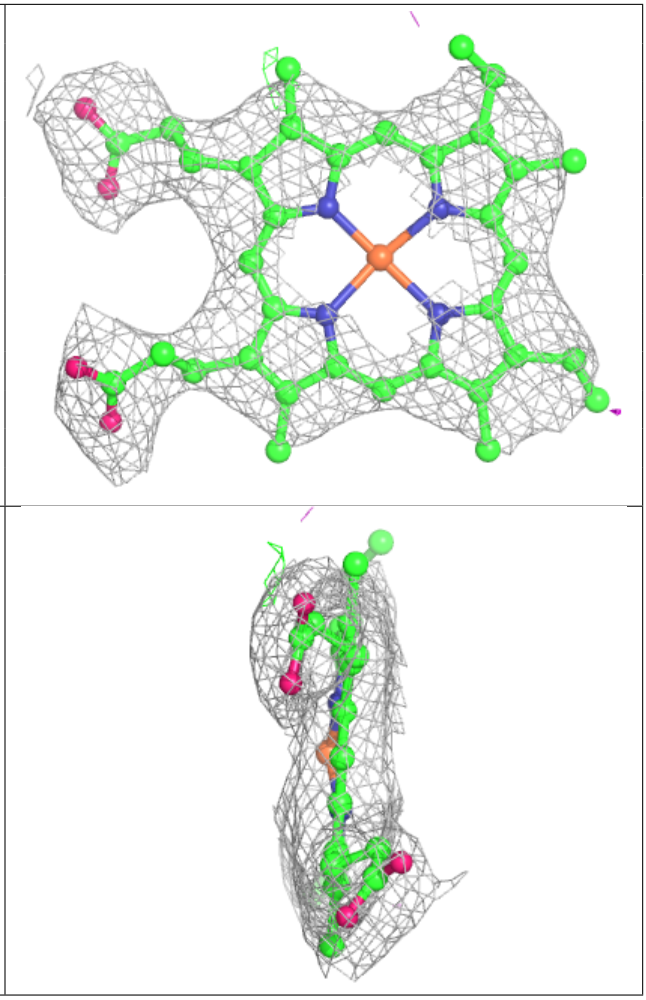
Electron density around HEM B 201:

$2mF_o$-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 V 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 (i)

There are no such residues in this entry.