



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2020 – 12:06 PM BST

PDB ID : 3CX5  
Title : Structure of complex III with bound cytochrome c in reduced state and definition of a minimal core interface for electron transfer.  
Authors : Solmaz, S.R.N.; Hunte, C.  
Deposited on : 2008-04-23  
Resolution : 1.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
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) : 2.13

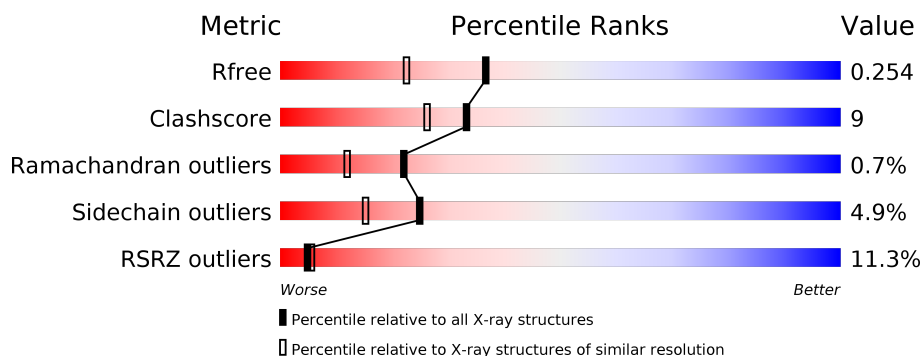
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	<div> <div>12%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	L	431	<div> <div>9%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>
2	B	352	<div> <div>8%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
2	M	352	<div> <div>10%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>
3	C	385	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
3	N	385	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	248	
4	O	248	
5	E	185	
5	P	185	
6	F	146	
6	Q	146	
7	G	126	
7	R	126	
8	H	93	
8	S	93	
9	I	65	
9	T	65	
10	J	127	
10	U	127	
11	K	107	
11	V	107	
12	W	108	
13	X	2	

## 2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 38020 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3344	2109	576	653	6			
1	L	431	Total	C	N	O	S	0	0	0
			3344	2109	576	653	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	conflict	UNP P07256
L	153	ASP	GLU	conflict	UNP P07256

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			
2	M	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	0	0	0
			3090	2082	484	503	21			
3	N	385	Total	C	N	O	S	0	0	0
			3090	2082	484	503	21			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	248	Total	C	N	O	S	0	0	0
			1961	1249	340	363	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	O	248	Total	C	N	O	S	0	0	0
			1961	1249	340	363	9			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			
5	P	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			
6	Q	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	126	Total	C	N	O	S	0	0	0
			1019	653	173	191	2			
7	R	126	Total	C	N	O	S	0	0	0
			1019	653	173	191	2			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	0	0	0
			773	510	131	130	2			
8	S	93	Total	C	N	O	S	0	0	0
			773	510	131	130	2			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	0	0	0
			465	310	77	78			
9	T	57	Total	C	N	O	0	0	0
			465	310	77	78			

- Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			
10	U	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			
11	V	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

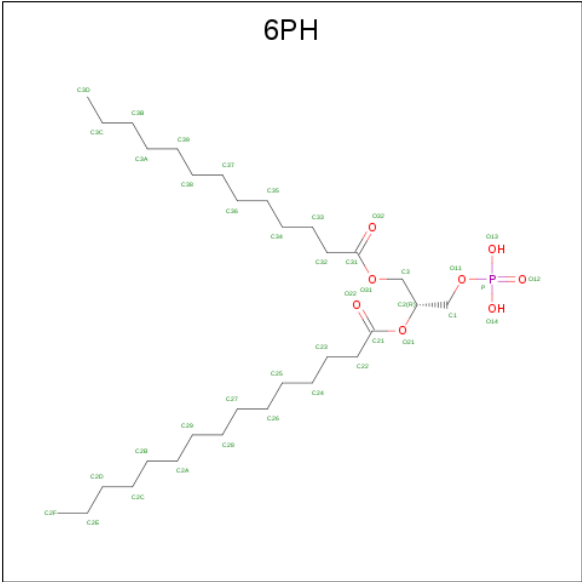
- Molecule 12 is a protein called Cytochrome c iso-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	108	Total	C	N	O	S	0	1	0
			859	542	153	159	5			

- Molecule 13 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.

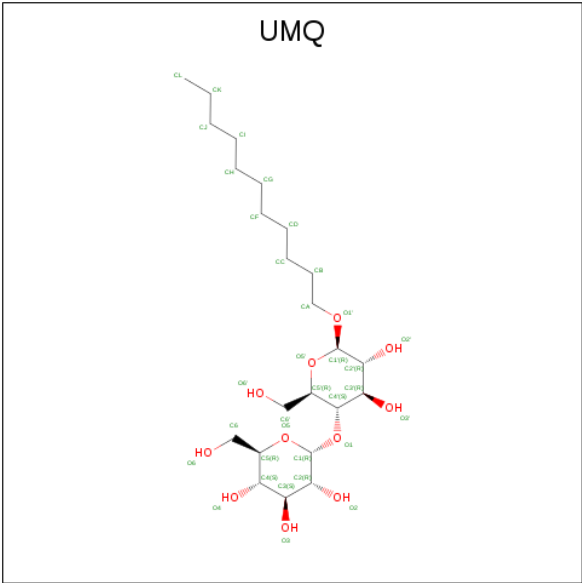
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
13	X	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 14 is (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (three-letter code: 6PH) (formula: C<sub>31</sub>H<sub>61</sub>O<sub>8</sub>P).



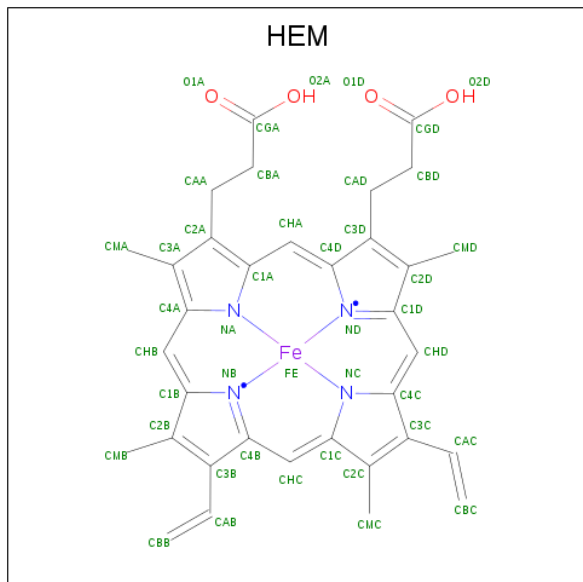
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	O	P	0	0
			40	31	8	1		
14	L	1	Total	C	O	P	0	0
			40	31	8	1		

- Molecule 15 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C<sub>23</sub>H<sub>44</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			34	23	11		
15	L	1	Total	C	O	0	0
			34	23	11		

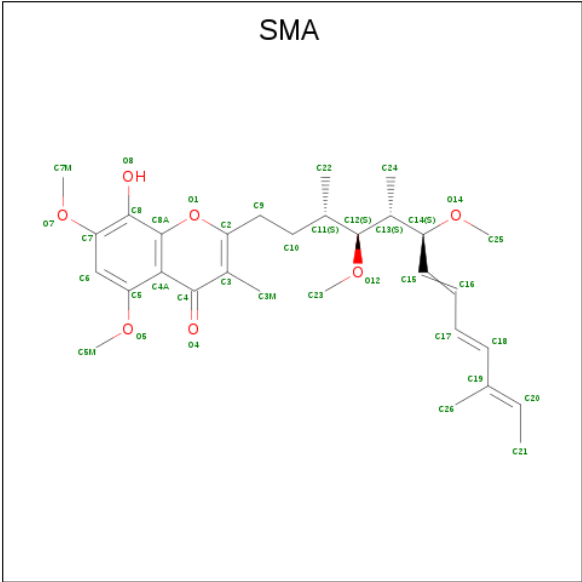
- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

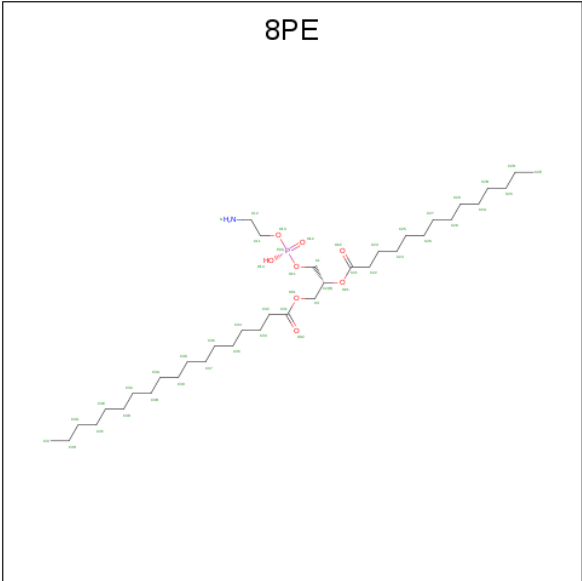
- Molecule 17 is STIGMATELLIN A (three-letter code: SMA) (formula:  $\text{C}_{30}\text{H}_{42}\text{O}_7$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			37	30	7		
17	N	1	Total	C	O	0	0
			37	30	7		

- Molecule 18 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (three-letter code: 8PE) (formula: C<sub>37</sub>H<sub>74</sub>NO<sub>8</sub>P).



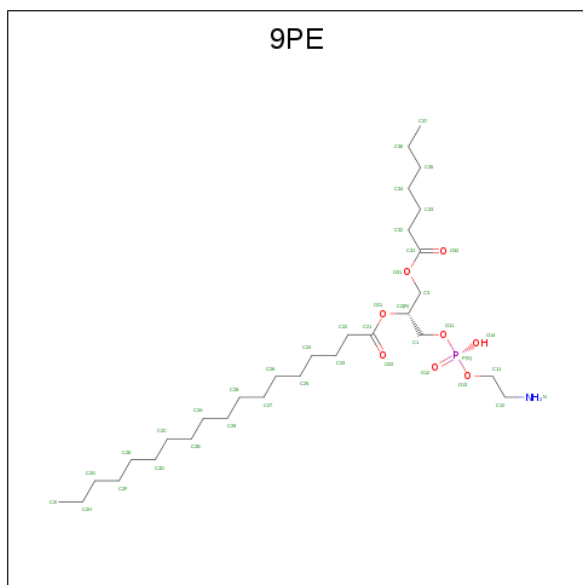
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

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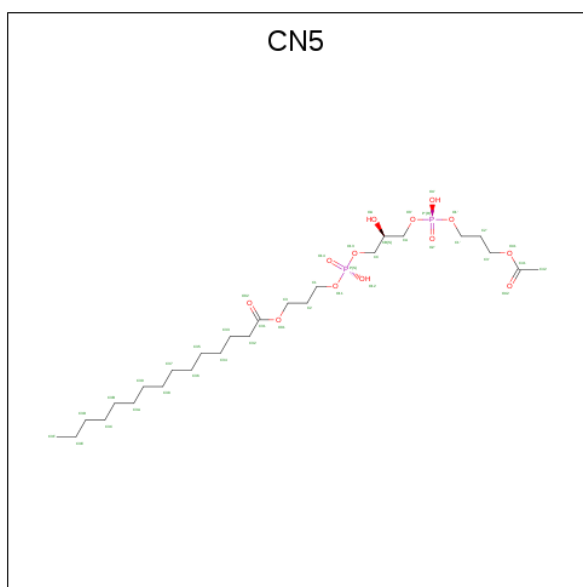
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	N	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

- Molecule 19 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (three-letter code: 9PE) (formula: C<sub>30</sub>H<sub>60</sub>NO<sub>8</sub>P).



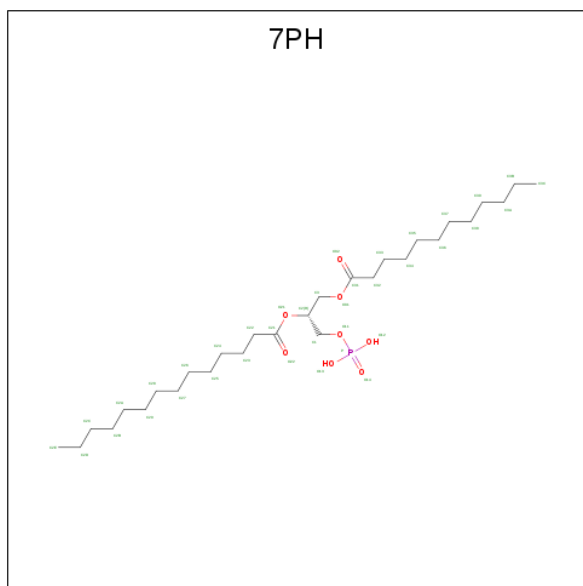
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
19	N	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 20 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-diphosphaoctadec-1-yl pentadecanoate (three-letter code: CN5) (formula: C<sub>26</sub>H<sub>52</sub>O<sub>13</sub>P<sub>2</sub>).



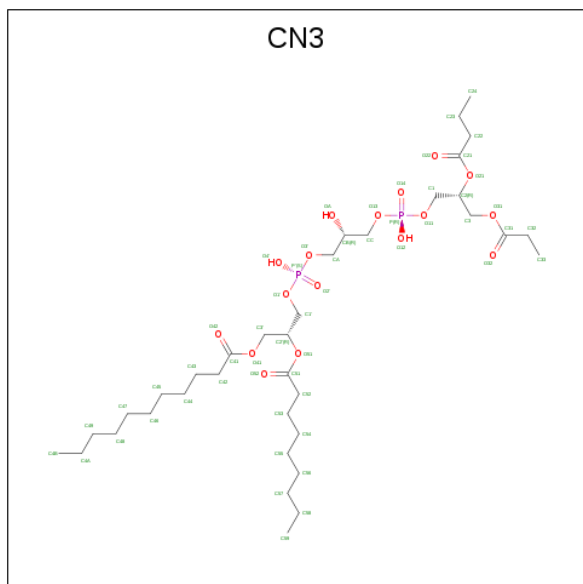
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	C	1	Total	C	O	P	0	0
			41	26	13	2		

- Molecule 21 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (three-letter code: 7PH) (formula:  $C_{29}H_{57}O_8P$ ).



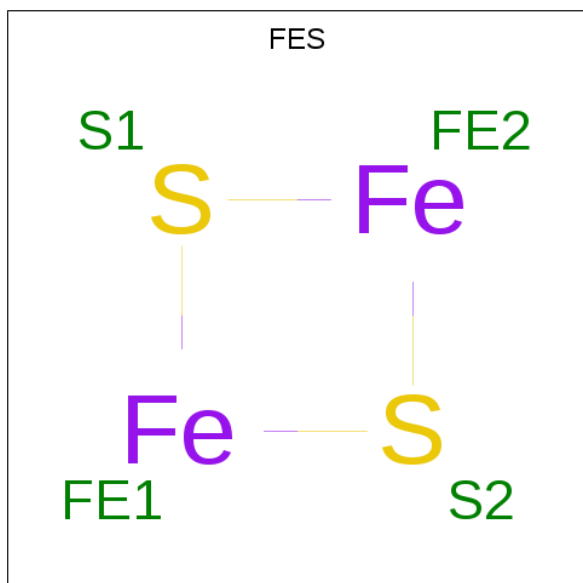
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	D	1	Total	C	O	P	0	0
			38	29	8	1		
21	O	1	Total	C	O	P	0	0
			38	29	8	1		

- Molecule 22 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanadec-1-yl undecanoate (three-letter code: CN3) (formula:  $C_{36}H_{68}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	D	1	Total	C	O	P	0	0
			55	36	17	2		
22	N	1	Total	C	O	P	0	0
			55	36	17	2		

- Molecule 23 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	E	1	Total	Fe	S	0	0
			4	2	2		
23	P	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	153	Total	O	0	0
			153	153		
24	B	93	Total	O	0	0
			93	93		
24	C	161	Total	O	0	0
			161	161		
24	D	154	Total	O	0	0
			154	154		
24	E	74	Total	O	0	0
			74	74		
24	F	16	Total	O	0	0
			16	16		
24	G	71	Total	O	0	0
			71	71		
24	H	31	Total	O	0	0
			31	31		
24	I	11	Total	O	0	0
			11	11		
24	J	15	Total	O	0	0
			15	15		
24	K	7	Total	O	0	0
			7	7		
24	L	170	Total	O	0	0
			170	170		
24	M	101	Total	O	0	0
			101	101		
24	N	170	Total	O	0	0
			170	170		
24	O	173	Total	O	0	0
			173	173		
24	P	66	Total	O	0	0
			66	66		
24	Q	27	Total	O	0	0
			27	27		
24	R	73	Total	O	0	0
			73	73		

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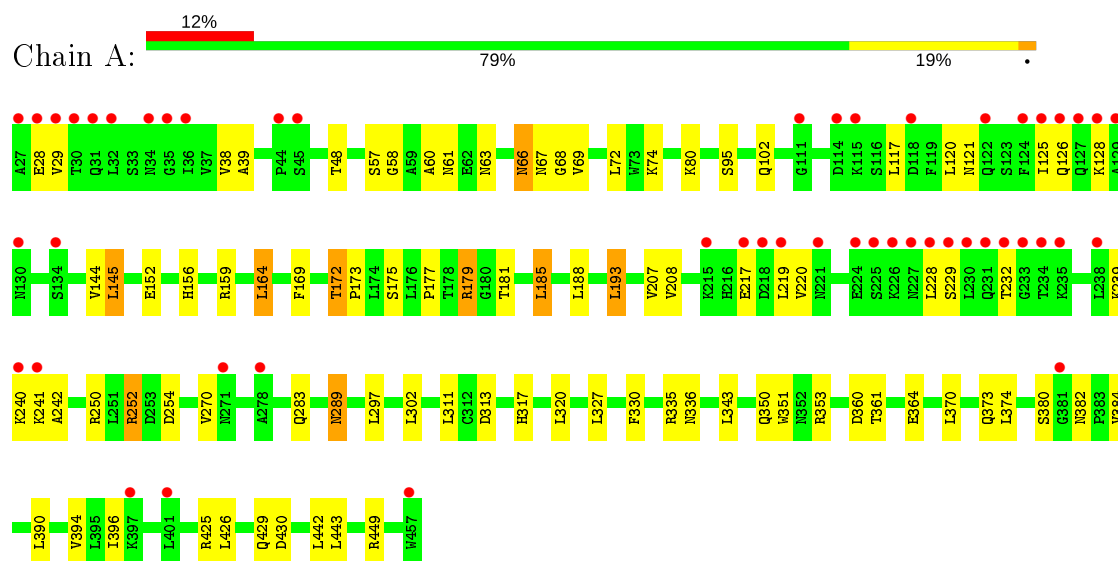
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	S	40	Total 40	O 40	0	0
24	T	12	Total 12	O 12	0	0
24	U	8	Total 8	O 8	0	0
24	V	2	Total 2	O 2	0	0
24	W	20	Total 20	O 20	0	0

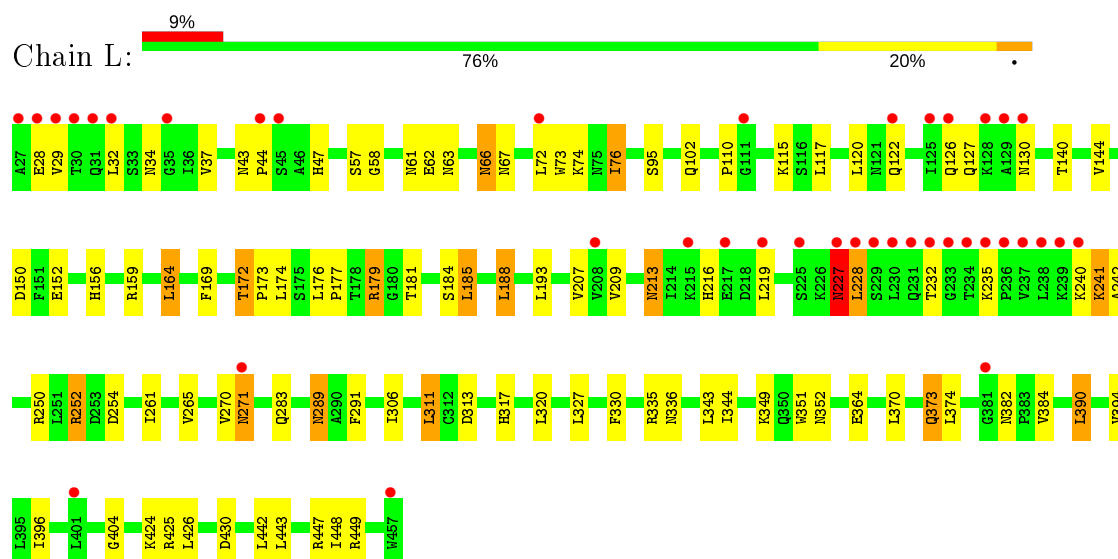
### 3 Residue-property plots [i](#)

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.

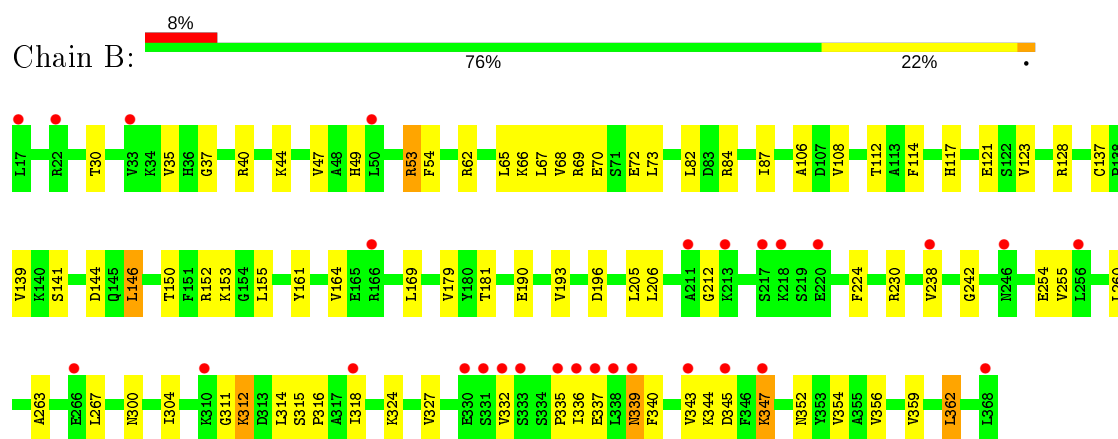
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



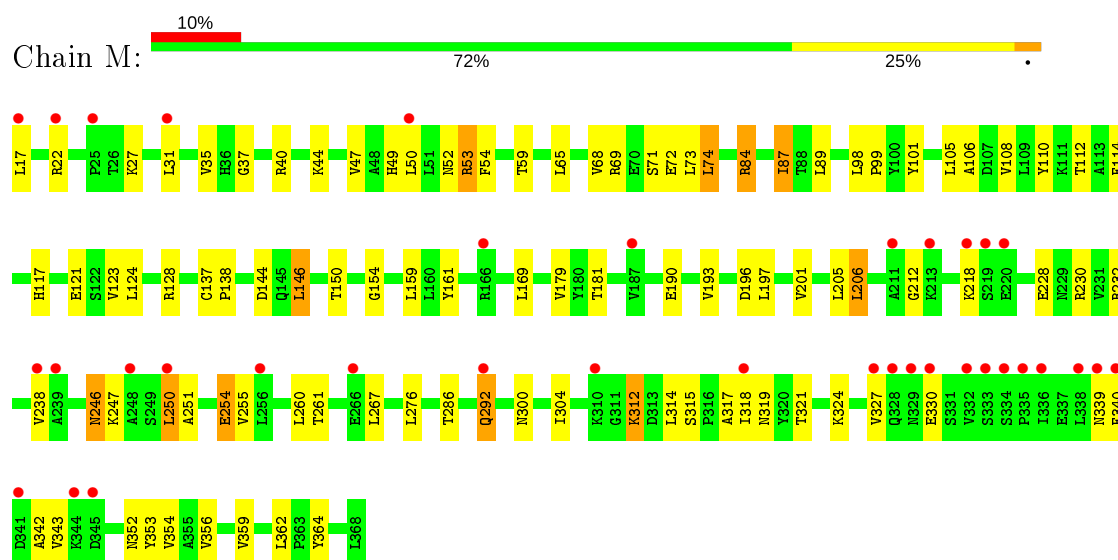
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



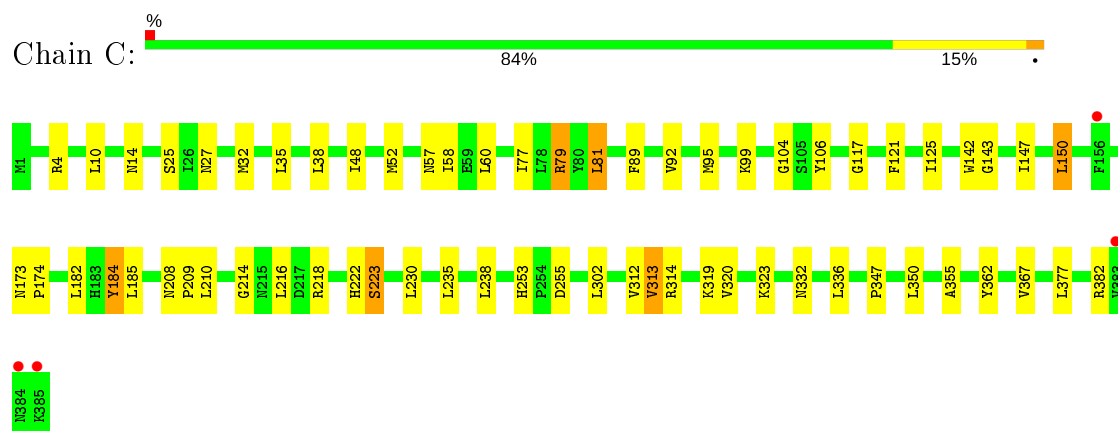
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



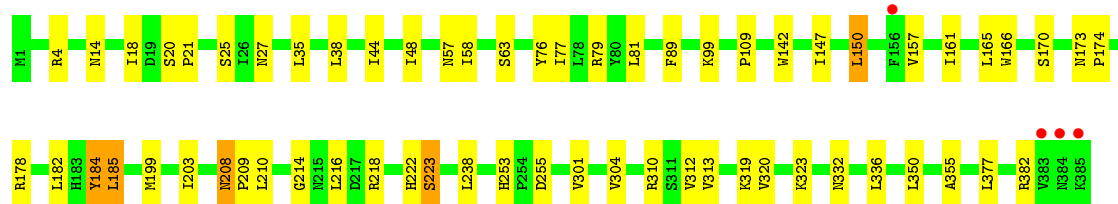
• Molecule 3: CYTOCHROME B



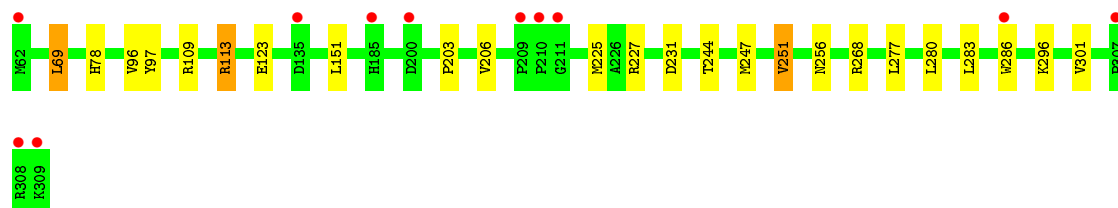
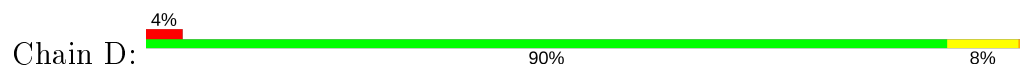
• Molecule 3: CYTOCHROME B







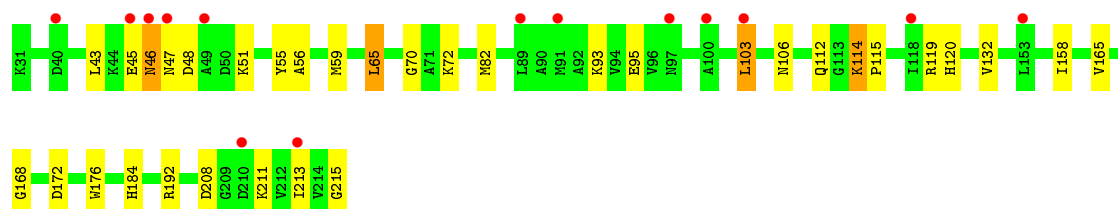
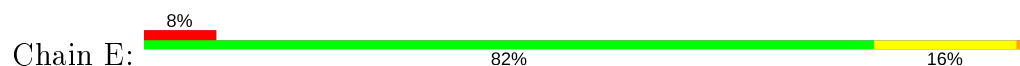
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



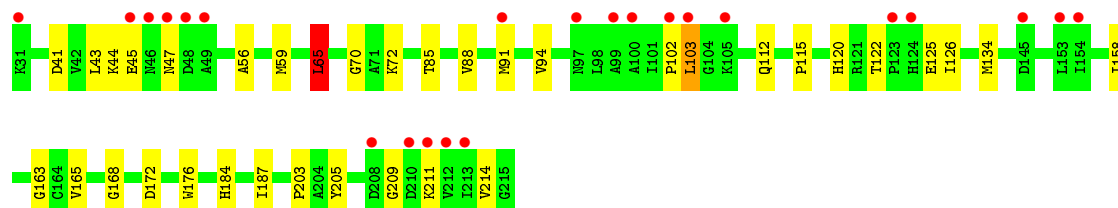
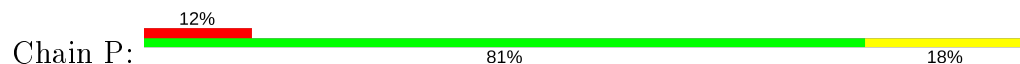
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

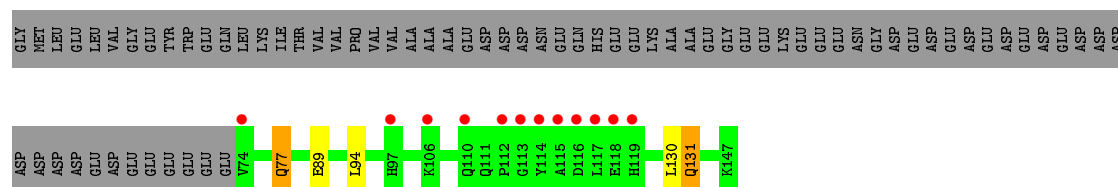


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

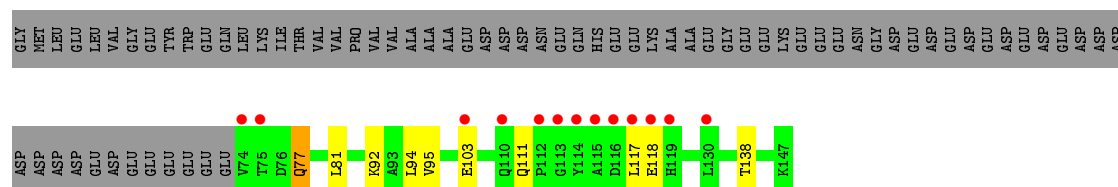
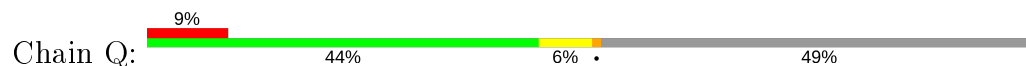


- Molecule 6: Cytochrome b-c1 complex subunit 6

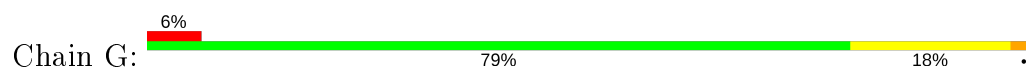




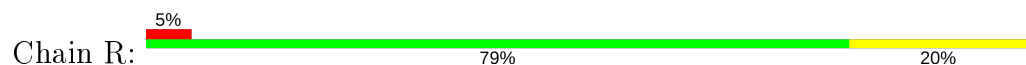
• Molecule 6: Cytochrome b-c1 complex subunit 6



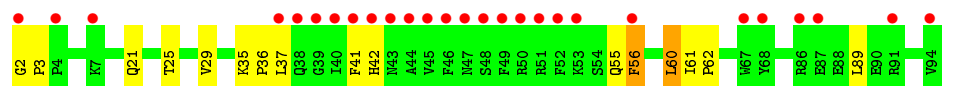
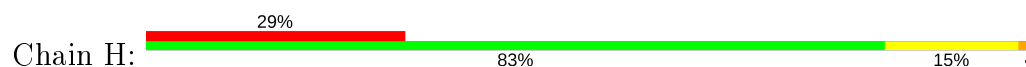
• Molecule 7: Cytochrome b-c1 complex subunit 7



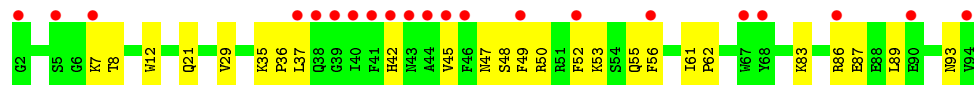
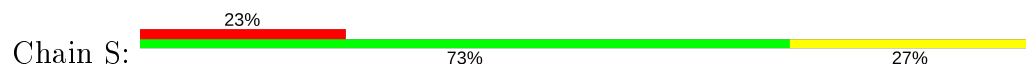
• Molecule 7: Cytochrome b-c1 complex subunit 7



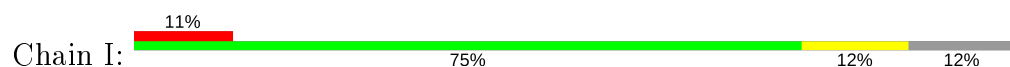
• Molecule 8: Cytochrome b-c1 complex subunit 8



• Molecule 8: Cytochrome b-c1 complex subunit 8

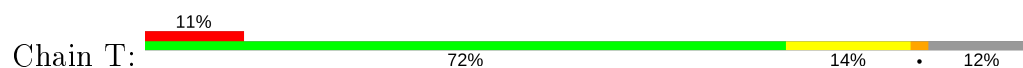


• Molecule 9: Cytochrome b-c1 complex subunit 9

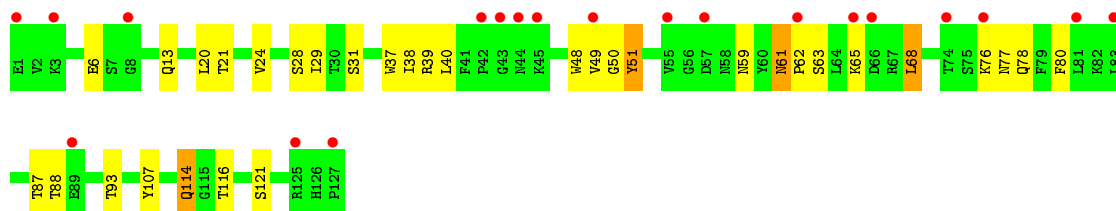
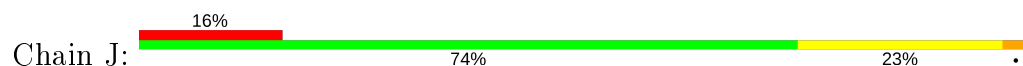




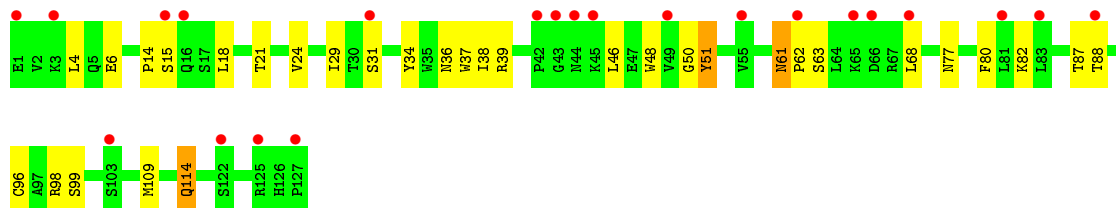
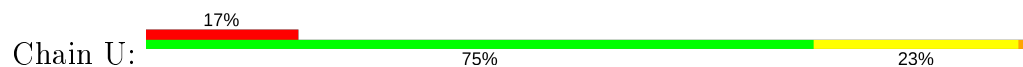
- Molecule 9: Cytochrome b-c1 complex subunit 9



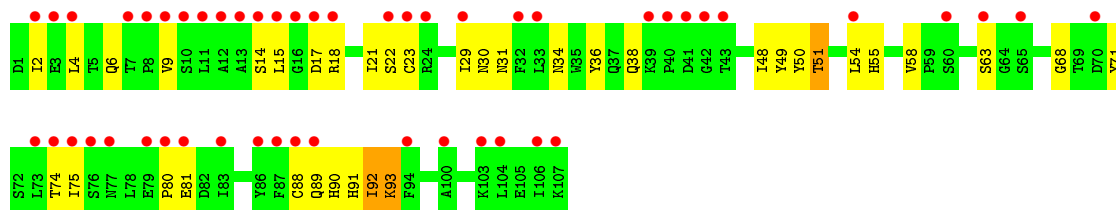
- Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT



- Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

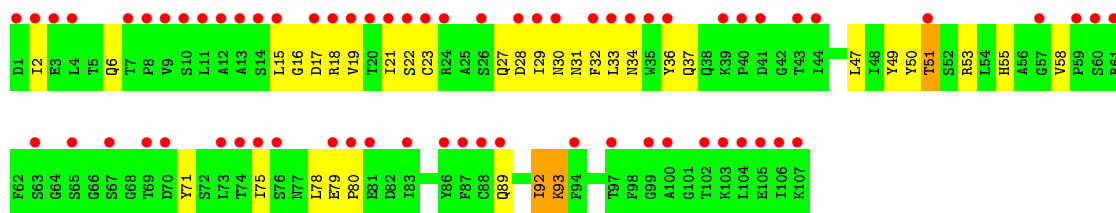


- Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

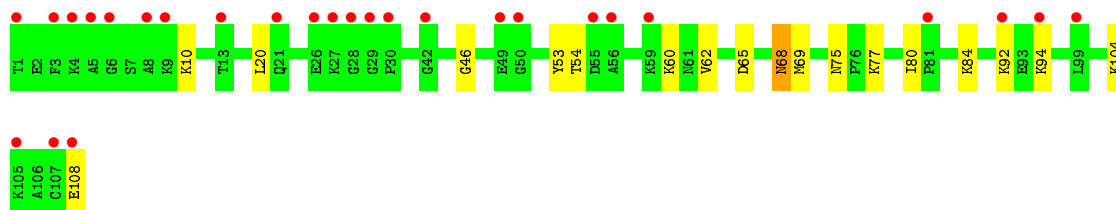
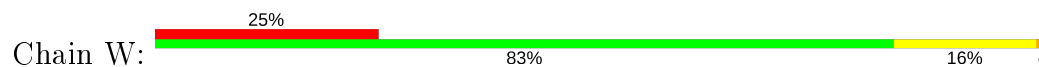


- Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT





● Molecule 12: Cytochrome c iso-1



● Molecule 13: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.12Å 165.09Å 194.37Å 90.00° 104.09° 90.00°	Depositor
Resolution (Å)	18.99 – 1.90 18.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (18.99-1.90) 95.2 (18.99-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.245 , 0.263 0.238 , 0.254	Depositor DCC
$R_{free}$ test set	33007 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	38020	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CN5, UMQ, CN3, GLC, 8PE, M3L, 7PH, FES, FRU, 9PE, HEM, 6PH, SMA

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	0.34	0/3405	0.60	0/4614
1	L	0.35	0/3405	0.60	1/4614 (0.0%)
2	B	0.33	0/2781	0.60	1/3764 (0.0%)
2	M	0.34	0/2781	0.61	1/3764 (0.0%)
3	C	0.42	0/3192	0.63	1/4354 (0.0%)
3	N	0.43	0/3192	0.62	0/4354
4	D	0.36	0/2022	0.60	0/2751
4	O	0.37	0/2022	0.61	0/2751
5	E	0.34	0/1444	0.58	1/1957 (0.1%)
5	P	0.34	0/1444	0.58	2/1957 (0.1%)
6	F	0.33	0/638	0.49	0/858
6	Q	0.34	0/638	0.49	0/858
7	G	0.33	0/1040	0.60	1/1408 (0.1%)
7	R	0.36	0/1040	0.61	1/1408 (0.1%)
8	H	0.38	0/804	0.51	0/1088
8	S	0.37	0/804	0.53	0/1088
9	I	0.39	0/479	0.46	0/646
9	T	0.41	0/479	0.50	0/646
10	J	0.33	0/1043	0.60	0/1422
10	U	0.33	0/1043	0.59	0/1422
11	K	0.31	0/863	0.50	0/1172
11	V	0.30	0/863	0.51	0/1172
12	W	0.31	0/865	0.54	0/1157
All	All	0.36	0/36287	0.59	9/49225 (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
4	D	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	314	ARG	NE-CZ-NH1	-6.89	116.85	120.30
2	M	87	ILE	N-CA-C	-6.26	94.09	111.00
2	B	87	ILE	N-CA-C	-5.98	94.86	111.00
5	E	65	LEU	CA-CB-CG	5.74	128.49	115.30
7	R	71	ARG	NE-CZ-NH1	-5.70	117.45	120.30
5	P	65	LEU	CA-CB-CG	5.60	128.18	115.30
5	P	163	GLY	N-CA-C	5.26	126.26	113.10
7	G	71	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	L	447	ARG	NE-CZ-NH1	-5.12	117.74	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	97	TYR	Sidechain

## 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	3344	0	3321	62	0
1	L	3344	0	3321	76	0
2	B	2735	0	2774	69	0
2	M	2735	0	2774	70	0
3	C	3090	0	3129	43	0
3	N	3090	0	3129	40	0
4	D	1961	0	1888	21	0
4	O	1961	0	1888	16	0
5	E	1411	0	1386	28	0
5	P	1411	0	1386	27	0
6	F	624	0	581	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	624	0	581	6	0
7	G	1019	0	1034	22	0
7	R	1019	0	1034	19	0
8	H	773	0	736	10	0
8	S	773	0	736	18	0
9	I	465	0	459	7	0
9	T	465	0	459	9	0
10	J	1015	0	959	29	0
10	U	1015	0	959	25	0
11	K	842	0	820	28	0
11	V	842	0	820	25	0
12	W	859	0	862	13	0
13	X	23	0	21	5	0
14	A	40	0	59	1	0
14	L	40	0	59	3	0
15	A	34	0	44	2	0
15	L	34	0	44	2	0
16	C	86	0	60	2	0
16	D	43	0	30	1	0
16	N	86	0	60	3	0
16	O	43	0	30	0	0
16	W	43	0	30	0	0
17	C	37	0	42	1	0
17	N	37	0	42	0	0
18	C	47	0	73	1	0
18	N	47	0	73	0	0
19	C	40	0	59	0	0
19	N	40	0	59	0	0
20	C	41	0	50	5	0
21	D	38	0	55	2	0
21	O	38	0	55	2	0
22	D	55	0	66	5	0
22	N	55	0	66	5	0
23	E	4	0	0	0	0
23	P	4	0	0	0	0
24	A	153	0	0	2	0
24	B	93	0	0	8	0
24	C	161	0	0	2	0
24	D	154	0	0	5	0
24	E	74	0	0	0	0
24	F	16	0	0	0	0
24	G	71	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	H	31	0	0	0	0
24	I	11	0	0	0	0
24	J	15	0	0	0	0
24	K	7	0	0	0	0
24	L	170	0	0	0	0
24	M	101	0	0	1	0
24	N	170	0	0	1	0
24	O	173	0	0	6	0
24	P	66	0	0	2	0
24	Q	27	0	0	0	0
24	R	73	0	0	1	0
24	S	40	0	0	0	0
24	T	12	0	0	1	0
24	U	8	0	0	0	0
24	V	2	0	0	0	0
24	W	20	0	0	0	0
All	All	38020	0	36113	620	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 9.

All (620) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:THR:HG22	2:B:352:ASN:HD22	1.27	1.00
2:M:246:ASN:HD22	2:M:246:ASN:H	1.11	0.99
6:F:77:GLN:HE21	6:F:77:GLN:H	1.12	0.97
2:M:150:THR:HG22	2:M:352:ASN:HD22	1.27	0.97
2:M:255:VAL:HG12	2:M:321:THR:HG21	1.47	0.96
1:L:63:ASN:H	1:L:66:ASN:HD21	1.10	0.92
1:A:63:ASN:H	1:A:66:ASN:HD21	1.18	0.91
10:J:114:GLN:H	10:J:114:GLN:HE21	1.21	0.88
7:R:77:ARG:HD3	7:R:88:LEU:HD11	1.56	0.88
10:J:29:ILE:H	10:J:77:ASN:HD21	1.16	0.87
6:Q:77:GLN:H	6:Q:77:GLN:HE21	1.14	0.86
12:W:20:LEU:HD23	13:X:2:FRU:H12	1.58	0.86
2:B:318:ILE:HD11	2:B:340:PHE:HB3	1.59	0.84
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.60	0.84
11:K:31:ASN:HD22	11:K:51:THR:HG21	1.42	0.83
22:N:4131:CN3:HAA	7:R:85:HIS:NE2	1.93	0.83
2:B:150:THR:HG22	2:B:352:ASN:ND2	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:150:THR:HG22	2:M:352:ASN:ND2	1.92	0.83
1:A:361:THR:HG21	7:R:123:ILE:O	1.80	0.82
12:W:60:LYS:HG3	12:W:62:VAL:HG23	1.62	0.82
1:A:63:ASN:H	1:A:66:ASN:ND2	1.78	0.82
2:B:49:HIS:HD2	2:B:161:TYR:H	1.28	0.81
1:L:317:HIS:HE1	1:L:351:TRP:HE1	1.28	0.80
1:A:179:ARG:HG2	1:A:179:ARG:HH21	1.47	0.80
2:M:246:ASN:H	2:M:246:ASN:ND2	1.80	0.79
2:M:318:ILE:HD11	2:M:340:PHE:HB3	1.65	0.79
6:Q:77:GLN:H	6:Q:77:GLN:NE2	1.81	0.78
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.30	0.77
2:M:49:HIS:HD2	2:M:161:TYR:H	1.33	0.77
3:N:58:ILE:H	3:N:173:ASN:HD22	1.29	0.77
10:U:29:ILE:H	10:U:77:ASN:HD21	1.32	0.77
1:L:63:ASN:H	1:L:66:ASN:ND2	1.82	0.77
7:G:31:GLN:HA	7:G:31:GLN:HE21	1.50	0.77
6:F:77:GLN:NE2	6:F:77:GLN:H	1.82	0.76
4:O:225:MET:HE2	24:O:5654:HOH:O	1.85	0.76
1:A:58:GLY:H	1:A:61:ASN:HD22	1.32	0.76
22:D:4031:CN3:HAA	7:G:85:HIS:NE2	2.02	0.75
3:N:214:GLY:O	3:N:218:ARG:HD2	1.87	0.75
2:B:108:VAL:O	2:B:112:THR:HG23	1.86	0.75
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.69	0.75
2:B:238:VAL:HG13	2:B:356:VAL:HB	1.68	0.74
2:M:37:GLY:HA3	2:M:179:VAL:HG11	1.68	0.74
10:J:6:GLU:H	10:J:114:GLN:HE22	1.35	0.74
5:P:172:ASP:H	5:P:184:HIS:HD2	1.36	0.74
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.70	0.73
5:E:95:GLU:HG2	5:E:213:ILE:HG22	1.70	0.73
10:U:114:GLN:HE21	10:U:114:GLN:H	1.35	0.73
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.54	0.72
2:M:108:VAL:O	2:M:112:THR:HG23	1.87	0.72
3:C:58:ILE:H	3:C:173:ASN:HD22	1.36	0.72
2:B:62:ARG:HG2	2:B:62:ARG:HH21	1.54	0.71
1:L:32:LEU:HG	1:L:216:HIS:HE2	1.54	0.71
7:R:77:ARG:HD2	24:R:5803:HOH:O	1.91	0.70
3:N:253:HIS:HD2	3:N:255:ASP:H	1.38	0.70
5:P:115:PRO:HD2	5:P:158:ILE:HD11	1.73	0.70
11:K:6:GLN:HG2	11:K:23:CYS:SG	2.31	0.70
1:L:404:GLY:HA2	2:M:27:LYS:HE3	1.72	0.70
1:L:179:ARG:HH21	1:L:179:ARG:HG2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:283:GLN:NE2	1:L:373:GLN:HE21	1.90	0.70
2:M:324:LYS:O	2:M:327:VAL:HG22	1.93	0.69
2:B:260:LEU:HD22	2:B:267:LEU:HD11	1.72	0.69
7:G:125:VAL:HG21	1:L:364:GLU:HG3	1.73	0.69
3:C:312:VAL:HG21	7:G:5:PHE:CE1	2.28	0.68
3:C:253:HIS:HD2	3:C:255:ASP:H	1.41	0.68
3:N:323:LYS:NZ	8:S:55:GLN:HE22	1.91	0.68
2:B:62:ARG:NH2	2:B:67:LEU:HD13	2.08	0.67
11:V:2:ILE:H	11:V:2:ILE:HD12	1.59	0.67
2:M:238:VAL:HG13	2:M:356:VAL:HB	1.75	0.67
5:P:172:ASP:H	5:P:184:HIS:CD2	2.11	0.67
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.42	0.67
2:B:300:ASN:O	2:B:304:ILE:HG12	1.95	0.66
2:M:300:ASN:O	2:M:304:ILE:HG12	1.95	0.66
4:D:227:ARG:HH11	4:D:244:THR:HG21	1.59	0.66
2:M:260:LEU:HD22	2:M:267:LEU:HD11	1.78	0.66
1:L:117:LEU:HD11	1:L:219:LEU:HD12	1.76	0.66
3:N:44:ILE:O	3:N:48:ILE:HG12	1.94	0.66
1:L:317:HIS:CE1	1:L:351:TRP:HE1	2.13	0.66
12:W:65:ASP:H	12:W:68:ASN:HD21	1.44	0.66
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.13	0.65
1:A:382:ASN:OD1	1:A:384:VAL:HG22	1.96	0.65
11:V:36:TYR:HE2	11:V:89:GLN:HG2	1.60	0.65
20:C:4033:CN5:H3CA	14:L:4113:6PH:H2E	1.79	0.65
1:L:58:GLY:H	1:L:61:ASN:HD22	1.45	0.65
1:L:207:VAL:HG11	1:L:394:VAL:HG21	1.80	0.64
2:B:49:HIS:CD2	2:B:161:TYR:H	2.14	0.64
2:M:31:LEU:HD12	2:M:105:LEU:HD12	1.79	0.64
3:C:320:VAL:HG23	24:C:7051:HOH:O	1.97	0.64
2:B:137:CYS:SG	24:B:8522:HOH:O	2.55	0.64
1:L:122:GLN:HA	1:L:126:GLN:HB3	1.79	0.63
2:M:247:LYS:O	2:M:250:LEU:HD22	1.98	0.63
1:L:72:LEU:HD23	1:L:193:LEU:HD21	1.80	0.63
5:P:91:MET:HG2	5:P:112:GLN:NE2	2.14	0.63
1:L:72:LEU:HB3	1:L:193:LEU:HD11	1.79	0.63
10:U:21:THR:HG22	10:U:80:PHE:HD2	1.63	0.63
1:A:68:GLY:HA3	1:A:185:LEU:HD11	1.81	0.63
1:L:72:LEU:HD22	1:L:188:LEU:HD23	1.79	0.62
2:B:164:VAL:HG21	2:M:232:ARG:HH11	1.63	0.62
4:O:213:ASN:OD1	13:X:2:FRU:H62	1.99	0.62
4:D:113:ARG:HG2	4:D:151:LEU:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:134:MET:HG3	10:U:31:SER:HB3	1.81	0.62
5:E:172:ASP:H	5:E:184:HIS:HD2	1.47	0.62
5:E:48:ASP:HB3	5:E:51:LYS:HG2	1.80	0.62
3:C:208:ASN:HD22	3:C:210:LEU:H	1.47	0.62
4:O:113:ARG:NE	24:O:6841:HOH:O	2.27	0.62
2:B:146:LEU:O	2:B:150:THR:HG23	2.00	0.62
20:C:4033:CN5:H3E	14:L:4113:6PH:H2B	1.82	0.62
2:M:65:LEU:O	2:M:69:ARG:HG2	1.99	0.62
10:U:6:GLU:H	10:U:114:GLN:HE22	1.48	0.62
1:A:121:ASN:ND2	1:A:125:ILE:HD12	2.14	0.61
7:G:77:ARG:HD2	24:G:5303:HOH:O	1.99	0.61
2:B:336:ILE:HD12	2:B:336:ILE:H	1.64	0.61
3:C:27:ASN:HB2	22:D:4031:CN3:O2'	1.99	0.61
1:A:117:LEU:HD11	1:A:219:LEU:HD12	1.83	0.61
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.82	0.61
9:T:5:SER:O	9:T:9:THR:HG23	2.01	0.61
3:N:208:ASN:HD22	3:N:210:LEU:H	1.49	0.60
3:N:253:HIS:CD2	3:N:255:ASP:H	2.17	0.60
3:N:320:VAL:HG23	24:N:6971:HOH:O	2.02	0.60
10:U:29:ILE:HG12	10:U:77:ASN:ND2	2.16	0.60
10:J:28:SER:HB3	10:J:31:SER:OG	2.02	0.60
12:W:54:THR:CG2	12:W:84:LYS:HG3	2.31	0.60
1:A:72:LEU:HD23	1:A:193:LEU:HD21	1.83	0.60
2:M:71:SER:HA	2:M:74:LEU:CD1	2.32	0.59
3:N:58:ILE:H	3:N:173:ASN:ND2	1.99	0.59
9:T:8:LYS:O	9:T:12:LYS:HD2	2.02	0.59
3:C:4:ARG:HE	3:C:14:ASN:ND2	2.00	0.59
3:C:52:MET:CE	5:E:82:MET:HG2	2.32	0.59
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.83	0.59
10:J:29:ILE:HG12	10:J:77:ASN:ND2	2.18	0.59
12:W:20:LEU:HD23	13:X:2:FRU:C1	2.31	0.59
3:N:27:ASN:HB2	22:N:4131:CN3:O2'	2.02	0.59
11:V:79:GLU:HB3	11:V:80:PRO:HD3	1.84	0.59
2:B:193:VAL:HG23	2:B:196:ASP:HB2	1.85	0.59
1:L:72:LEU:CD1	1:L:144:VAL:HG21	2.33	0.59
1:A:179:ARG:NH2	1:A:179:ARG:HG2	2.14	0.59
2:B:30:THR:CG2	2:B:190:GLU:HB3	2.33	0.59
1:L:252:ARG:HD3	1:L:254:ASP:OD1	2.03	0.59
4:D:227:ARG:NH1	4:D:244:THR:HG21	2.18	0.58
10:J:24:VAL:HG21	10:J:29:ILE:HD11	1.85	0.58
10:J:29:ILE:H	10:J:77:ASN:ND2	1.94	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:83:LYS:O	8:S:86:ARG:HG2	2.04	0.58
1:L:241:LYS:HD2	1:L:241:LYS:H	1.68	0.58
1:A:217:GLU:HA	1:A:220:VAL:HG12	1.86	0.58
1:A:228:LEU:HG	1:A:229:SER:H	1.67	0.58
2:B:121:GLU:OE2	7:R:62:ARG:HD2	2.04	0.58
8:H:56:PHE:O	8:H:60:LEU:HB2	2.03	0.58
1:L:156:HIS:HD2	1:L:159:ARG:HH21	1.51	0.58
3:C:253:HIS:CD2	3:C:255:ASP:H	2.21	0.58
1:A:283:GLN:HE22	1:A:373:GLN:HE21	1.52	0.58
3:C:214:GLY:O	3:C:218:ARG:HD2	2.03	0.58
6:F:77:GLN:HE21	6:F:77:GLN:N	1.93	0.58
4:D:247:MET:O	4:D:251:VAL:HG22	2.05	0.57
11:K:36:TYR:CE2	11:K:89:GLN:HG2	2.37	0.57
1:A:429:GLN:HE22	9:I:13:ARG:HH21	1.50	0.57
16:N:4022:HEM:HMC2	16:N:4022:HEM:HBC2	1.85	0.57
7:G:97:GLN:NE2	7:G:97:GLN:H	2.03	0.57
2:M:181:THR:HB	2:M:212:GLY:H	1.70	0.57
2:B:315:SER:OG	2:B:344:LYS:HD2	2.04	0.57
7:G:53:ASN:ND2	7:G:56:MET:H	2.03	0.57
7:G:63:LEU:HD12	7:G:64:PRO:HD2	1.87	0.56
7:G:91:ASN:H	7:G:91:ASN:ND2	2.02	0.56
1:A:283:GLN:NE2	1:A:373:GLN:HE21	2.03	0.56
2:B:117:HIS:HB3	7:R:62:ARG:HG2	1.88	0.56
10:J:114:GLN:H	10:J:114:GLN:NE2	1.96	0.56
1:L:110:PRO:HB3	1:L:213:ASN:HB3	1.87	0.56
2:M:49:HIS:CD2	2:M:161:TYR:H	2.20	0.56
2:B:347:LYS:N	2:B:347:LYS:HD3	2.20	0.56
2:M:110:TYR:CD2	2:M:205:LEU:HD23	2.41	0.56
2:M:35:VAL:CG1	2:M:179:VAL:HG12	2.36	0.56
2:B:164:VAL:CG2	2:M:232:ARG:HH11	2.18	0.56
5:P:103:LEU:O	5:P:120:HIS:HB3	2.06	0.56
3:N:313:VAL:HG22	3:N:319:LYS:HE3	1.87	0.56
2:B:53:ARG:HB3	2:B:123:VAL:HG13	1.89	0.55
10:U:61:ASN:HD22	10:U:63:SER:H	1.52	0.55
2:B:30:THR:HG22	2:B:190:GLU:HB3	1.87	0.55
3:C:313:VAL:HG22	3:C:319:LYS:HE3	1.88	0.55
3:C:52:MET:HE1	5:E:82:MET:HG2	1.88	0.55
1:L:270:VAL:O	1:L:271:ASN:HB2	2.05	0.55
15:A:4021:UMQ:HC1	9:I:18:VAL:HG12	1.88	0.55
1:A:58:GLY:H	1:A:61:ASN:ND2	2.02	0.55
22:D:4031:CN3:HAA	7:G:85:HIS:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:20:LEU:HD22	10:J:116:THR:HG21	1.89	0.55
10:J:65:LYS:HA	10:J:68:LEU:HD11	1.87	0.55
3:N:4:ARG:HE	3:N:14:ASN:ND2	2.04	0.55
10:U:29:ILE:H	10:U:77:ASN:ND2	2.02	0.55
5:E:172:ASP:H	5:E:184:HIS:CD2	2.25	0.55
5:P:72:LYS:NZ	9:T:29:GLN:HE22	2.04	0.55
12:W:20:LEU:CD2	13:X:2:FRU:H12	2.34	0.55
11:V:29:ILE:HG22	11:V:92:ILE:HD12	1.88	0.55
2:M:193:VAL:HG23	2:M:196:ASP:HB2	1.88	0.55
3:N:57:ASN:HA	3:N:173:ASN:HD21	1.71	0.55
5:P:103:LEU:HG	5:P:122:THR:HG22	1.88	0.55
5:P:72:LYS:HZ3	9:T:29:GLN:HE22	1.55	0.54
5:E:51:LYS:HD3	9:I:4:SER:HB2	1.88	0.54
5:P:91:MET:HG2	5:P:112:GLN:HE21	1.70	0.54
3:N:323:LYS:CE	8:S:55:GLN:HE22	2.21	0.54
7:R:53:ASN:ND2	7:R:56:MET:H	2.05	0.54
1:L:169:PHE:O	1:L:172:THR:HB	2.08	0.54
11:V:37:GLN:HB2	11:V:47:LEU:HD11	1.89	0.54
10:J:21:THR:HG22	10:J:80:PHE:HD2	1.73	0.54
11:K:55:HIS:O	11:K:58:VAL:HG22	2.08	0.54
6:Q:81:LEU:HB3	6:Q:138:THR:HG22	1.89	0.54
2:B:44:LYS:O	2:B:47:VAL:HG23	2.07	0.54
3:N:147:ILE:HA	3:N:150:LEU:HD22	1.90	0.54
2:B:336:ILE:HG21	2:B:339:ASN:HD22	1.73	0.54
3:N:208:ASN:HB2	3:N:209:PRO:HD2	1.91	0.53
3:C:58:ILE:H	3:C:173:ASN:ND2	2.05	0.53
1:L:179:ARG:NH2	1:L:179:ARG:HG2	2.23	0.53
1:L:67:ASN:HD21	1:L:177:PRO:HG2	1.74	0.53
11:V:55:HIS:O	11:V:58:VAL:HG22	2.09	0.53
1:A:164:LEU:HD13	1:A:327:LEU:HD13	1.91	0.53
1:L:313:ASP:OD1	1:L:335:ARG:HD3	2.09	0.53
3:C:32:MET:HE2	3:C:95:MET:SD	2.48	0.53
5:E:213:ILE:HG13	5:E:213:ILE:O	2.08	0.53
7:R:63:LEU:HD12	7:R:64:PRO:HD2	1.91	0.53
7:G:62:ARG:HD2	2:M:121:GLU:OE2	2.08	0.53
2:M:71:SER:HA	2:M:74:LEU:HD11	1.89	0.53
8:S:89:LEU:O	8:S:93:ASN:HB2	2.08	0.53
1:A:207:VAL:HG11	1:A:394:VAL:HG21	1.90	0.53
1:L:382:ASN:OD1	1:L:384:VAL:HG22	2.08	0.53
1:A:302:LEU:HB2	1:A:350:GLN:HG3	1.91	0.53
2:M:53:ARG:HB3	2:M:123:VAL:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:14:PRO:O	10:U:15:SER:HB3	2.09	0.53
1:L:130:ASN:HD22	1:L:130:ASN:H	1.57	0.53
2:M:251:ALA:HB2	2:M:339:ASN:HB2	1.91	0.53
2:M:255:VAL:HG11	2:M:343:VAL:HG21	1.91	0.53
4:O:286:TRP:CE3	5:P:59:MET:HG3	2.44	0.53
12:W:104:LYS:O	12:W:108:GLU:HG2	2.08	0.53
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.90	0.53
2:M:255:VAL:HG23	2:M:314:LEU:HD13	1.91	0.53
2:M:292:GLN:NE2	2:M:292:GLN:H	2.06	0.53
2:B:238:VAL:CG1	2:B:356:VAL:HB	2.36	0.52
2:M:246:ASN:ND2	2:M:246:ASN:N	2.52	0.52
3:N:184:TYR:CD1	16:N:4021:HEM:HBC1	2.44	0.52
8:S:61:ILE:HB	8:S:62:PRO:HD3	1.91	0.52
10:U:87:THR:HG22	10:U:88:THR:N	2.24	0.52
10:U:61:ASN:ND2	10:U:63:SER:H	2.06	0.52
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.90	0.52
2:M:146:LEU:O	2:M:150:THR:HG23	2.09	0.52
2:B:65:LEU:HD11	2:B:69:ARG:NH2	2.23	0.52
1:L:306:ILE:HA	1:L:311:LEU:HD22	1.92	0.52
1:A:350:GLN:HE22	1:A:353:ARG:HH21	1.57	0.52
2:B:35:VAL:CG1	2:B:179:VAL:HG12	2.39	0.52
2:M:238:VAL:CG1	2:M:356:VAL:HB	2.39	0.52
11:V:34:ASN:HD22	11:V:49:TYR:HA	1.75	0.52
2:B:311:GLY:O	2:B:312:LYS:HD2	2.09	0.52
7:G:81:THR:HG22	7:G:86:HIS:O	2.10	0.52
4:O:78:HIS:HD2	24:O:5586:HOH:O	1.91	0.52
6:Q:77:GLN:N	6:Q:77:GLN:HE21	1.94	0.52
1:L:66:ASN:HA	1:L:188:LEU:HD11	1.90	0.52
2:M:106:ALA:HA	2:M:206:LEU:HD13	1.92	0.52
1:L:76:ILE:HG23	1:L:140:THR:HG21	1.92	0.52
1:L:289:ASN:HD22	1:L:289:ASN:C	2.12	0.52
1:L:344:ILE:HG21	1:L:448:ILE:HD12	1.91	0.52
2:M:68:VAL:O	2:M:72:GLU:HG3	2.10	0.52
7:G:117:LYS:HE2	24:M:7272:HOH:O	2.09	0.52
2:M:146:LEU:HD23	2:M:286:THR:HG22	1.91	0.52
11:K:15:LEU:H	11:K:15:LEU:HD12	1.75	0.52
1:L:28:GLU:HG2	1:L:29:VAL:N	2.25	0.52
2:M:31:LEU:HD12	2:M:105:LEU:CD1	2.40	0.52
1:A:145:LEU:CD1	1:A:185:LEU:HB3	2.40	0.51
3:C:147:ILE:O	3:C:150:LEU:HB2	2.09	0.51
3:C:4:ARG:HE	3:C:14:ASN:HD21	1.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:222:HIS:O	3:N:223:SER:HB2	2.10	0.51
12:W:68:ASN:HD22	12:W:69:MET:N	2.08	0.51
4:D:286:TRP:CZ3	5:E:56:ALA:HA	2.45	0.51
1:L:181:THR:O	1:L:185:LEU:HB2	2.09	0.51
6:Q:117:LEU:O	6:Q:118:GLU:HG2	2.09	0.51
10:U:4:LEU:HG	10:U:24:VAL:HG22	1.91	0.51
21:D:4014:7PH:H35	5:E:70:GLY:HA3	1.93	0.51
7:G:13:ASP:HB3	7:G:17:LYS:HE3	1.93	0.51
3:N:310:ARG:HA	7:R:2:PRO:HB2	1.92	0.51
1:L:172:THR:CG2	1:L:242:ALA:HA	2.41	0.51
3:N:63:SER:OG	4:O:109:ARG:NH1	2.43	0.51
7:G:91:ASN:H	7:G:91:ASN:HD22	1.58	0.51
1:L:28:GLU:HG2	1:L:29:VAL:H	1.74	0.51
10:J:114:GLN:HE21	10:J:114:GLN:N	2.00	0.51
1:L:283:GLN:HE21	1:L:373:GLN:HE21	1.58	0.51
4:D:231:ASP:OD1	4:D:244:THR:HG23	2.10	0.51
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.44	0.50
4:D:225:MET:HB2	16:D:4003:HEM:C1D	2.46	0.50
8:S:52:PHE:O	8:S:56:PHE:HB3	2.12	0.50
20:C:4033:CN5:H1'A	20:C:4033:CN5:HB	1.92	0.50
1:L:240:LYS:HG2	1:L:241:LYS:N	2.26	0.50
2:M:261:THR:O	2:M:261:THR:HG22	2.11	0.50
1:A:313:ASP:OD1	1:A:335:ARG:HD3	2.12	0.50
7:G:62:ARG:HG2	2:M:117:HIS:HB3	1.92	0.50
1:L:67:ASN:HD22	1:L:181:THR:HG23	1.76	0.50
5:P:122:THR:O	5:P:126:ILE:HG13	2.10	0.50
4:O:289:LYS:HB2	8:S:37:LEU:HD13	1.92	0.50
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.42	0.50
10:U:38:ILE:HD12	10:U:46:LEU:HD22	1.92	0.50
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.12	0.50
3:C:79:ARG:NH1	24:C:6790:HOH:O	2.45	0.50
15:L:4121:UMQ:O1'	9:T:18:VAL:HG13	2.11	0.50
10:U:61:ASN:HD22	10:U:61:ASN:C	2.15	0.50
2:B:112:THR:HG22	24:B:6011:HOH:O	2.12	0.50
3:C:235:LEU:HD23	22:D:4031:CN3:H45	1.93	0.50
5:E:103:LEU:O	5:E:120:HIS:HB3	2.12	0.50
11:K:29:ILE:HD11	11:K:71:TYR:CE1	2.47	0.50
1:A:67:ASN:HD21	1:A:177:PRO:HG2	1.75	0.50
10:U:114:GLN:H	10:U:114:GLN:NE2	2.07	0.50
7:G:12:GLY:O	7:G:16:LEU:HD22	2.11	0.49
22:N:4131:CN3:HC	24:O:6998:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:241:LYS:H	1:L:241:LYS:CD	2.25	0.49
1:L:265:VAL:HG21	1:L:426:LEU:HD12	1.93	0.49
21:O:4114:7PH:H35	5:P:70:GLY:HA3	1.94	0.49
8:S:42:HIS:H	8:S:45:VAL:HG12	1.76	0.49
2:B:146:LEU:HD13	2:B:354:VAL:HG22	1.94	0.49
10:J:61:ASN:C	10:J:61:ASN:HD22	2.16	0.49
11:K:2:ILE:HD11	11:K:93:LYS:NZ	2.28	0.49
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.47	0.49
1:L:172:THR:HG23	1:L:242:ALA:HA	1.95	0.49
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.47	0.49
15:L:4121:UMQ:HC1	9:T:18:VAL:HG12	1.94	0.49
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.77	0.49
2:M:260:LEU:CD2	2:M:267:LEU:HD11	2.42	0.49
3:N:147:ILE:O	3:N:150:LEU:HB2	2.13	0.49
3:N:4:ARG:HE	3:N:14:ASN:HD21	1.58	0.49
11:K:2:ILE:HD12	11:K:2:ILE:N	2.27	0.49
1:A:297:LEU:O	2:B:69:ARG:NH2	2.40	0.49
1:L:270:VAL:HG21	1:L:396:ILE:HD13	1.94	0.49
1:A:229:SER:HB3	1:A:232:THR:HB	1.95	0.49
1:A:48:THR:HG21	2:B:327:VAL:HG12	1.95	0.48
4:D:109:ARG:NH2	24:D:6205:HOH:O	2.46	0.48
10:J:37:TRP:O	10:J:49:VAL:HB	2.13	0.48
11:K:34:ASN:HD22	11:K:49:TYR:HA	1.76	0.48
11:K:31:ASN:ND2	11:K:51:THR:HG21	2.21	0.48
1:A:289:ASN:HD22	1:A:289:ASN:C	2.16	0.48
4:D:78:HIS:HD2	24:D:5086:HOH:O	1.96	0.48
11:K:2:ILE:H	11:K:2:ILE:HD12	1.78	0.48
4:O:203:PRO:HG2	4:O:206:VAL:HG21	1.94	0.48
1:A:68:GLY:HA3	1:A:185:LEU:CD1	2.42	0.48
3:C:222:HIS:O	3:C:223:SER:HB2	2.12	0.48
11:V:17:ASP:O	11:V:78:LEU:HD13	2.14	0.48
11:V:53:ARG:HH21	11:V:53:ARG:HG3	1.77	0.48
1:A:250:ARG:NH1	1:A:442:LEU:O	2.47	0.48
11:V:47:LEU:HA	11:V:58:VAL:HG11	1.96	0.48
12:W:92:LYS:HD2	12:W:94:LYS:HE2	1.95	0.48
7:R:120:LEU:HA	7:R:123:ILE:HG23	1.94	0.48
12:W:60:LYS:HG2	12:W:80:ILE:HG12	1.94	0.48
5:E:93:LYS:HD3	5:E:215:GLY:HA3	1.95	0.48
10:J:29:ILE:N	10:J:77:ASN:HD21	1.98	0.48
11:V:19:VAL:HG12	11:V:75:ILE:HB	1.96	0.48
2:B:318:ILE:HG22	24:B:8526:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:ILE:CD1	2:B:340:PHE:HB3	2.39	0.48
11:K:18:ARG:HB2	11:K:75:ILE:O	2.14	0.48
1:L:250:ARG:NH1	1:L:442:LEU:O	2.47	0.48
5:P:125:GLU:HB3	5:P:187:ILE:HG12	1.95	0.48
1:A:252:ARG:HD2	8:H:21:GLN:HB2	1.94	0.47
5:P:214:VAL:N	24:P:7409:HOH:O	2.46	0.47
5:P:65:LEU:HD13	9:T:25:ALA:HA	1.96	0.47
1:L:66:ASN:H	1:L:66:ASN:HD22	1.63	0.47
3:N:332:ASN:HD21	3:N:355:ALA:HA	1.78	0.47
10:J:61:ASN:HD22	10:J:62:PRO:N	2.12	0.47
4:O:213:ASN:HB3	13:X:1:GLC:O4	2.14	0.47
3:C:184:TYR:CD1	16:C:4001:HEM:HBC1	2.49	0.47
11:V:50:TYR:O	11:V:51:THR:HG22	2.13	0.47
10:J:61:ASN:ND2	10:J:63:SER:H	2.13	0.47
20:C:4033:CN5:H3FB	14:L:4113:6PH:H29A	1.96	0.47
4:D:203:PRO:HG2	4:D:206:VAL:CG2	2.43	0.47
5:E:112:GLN:O	5:E:114:LYS:HD3	2.14	0.47
5:P:94:VAL:N	24:P:7409:HOH:O	2.46	0.47
2:B:40:ARG:HG3	2:B:155:LEU:HG	1.95	0.47
2:B:106:ALA:HA	2:B:206:LEU:HD13	1.96	0.47
3:C:147:ILE:HA	3:C:150:LEU:HD22	1.96	0.47
9:T:50:LYS:HG3	24:T:6999:HOH:O	2.13	0.47
3:C:323:LYS:HE3	8:H:55:GLN:HE22	1.80	0.47
10:U:36:ASN:OD1	10:U:51:TYR:HB3	2.15	0.47
11:V:34:ASN:ND2	11:V:49:TYR:HA	2.29	0.47
11:K:21:ILE:HG22	11:K:22:SER:N	2.30	0.47
11:K:90:HIS:HD2	11:K:92:ILE:HG22	1.80	0.47
2:M:230:ARG:HE	2:M:359:VAL:HG13	1.80	0.47
6:Q:92:LYS:HA	6:Q:95:VAL:HG22	1.96	0.47
2:B:324:LYS:O	2:B:327:VAL:HG22	2.14	0.47
4:D:268:ARG:NH1	9:I:33:ASP:OD1	2.48	0.47
10:J:51:TYR:CD2	10:J:51:TYR:C	2.89	0.47
11:K:34:ASN:HD21	11:K:91:HIS:HE1	1.63	0.47
1:L:172:THR:HG23	1:L:173:PRO:HD2	1.97	0.47
1:L:164:LEU:HD13	1:L:327:LEU:HD13	1.97	0.47
2:B:139:VAL:HG22	24:B:8522:HOH:O	2.15	0.47
5:E:132:VAL:HG21	5:E:192:ARG:NH1	2.30	0.47
4:D:69:LEU:HD11	6:F:131:GLN:HB3	1.96	0.47
5:P:43:LEU:HD21	8:S:29:VAL:HG11	1.97	0.47
11:V:19:VAL:HG12	11:V:78:LEU:HD11	1.97	0.47
2:B:152:ARG:HD3	2:B:224:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:GLY:O	3:C:147:ILE:HG12	2.15	0.46
9:I:3:PHE:CE1	9:I:5:SER:HB2	2.50	0.46
10:J:48:TRP:CZ2	10:J:50:GLY:HA2	2.50	0.46
2:B:49:HIS:HA	2:B:82:LEU:HD22	1.98	0.46
2:B:205:LEU:HD23	24:B:7883:HOH:O	2.16	0.46
5:P:65:LEU:CD1	9:T:25:ALA:HA	2.45	0.46
3:C:77:ILE:O	3:C:81:LEU:HB2	2.15	0.46
4:D:296:LYS:HE3	24:D:5128:HOH:O	2.15	0.46
5:E:43:LEU:HD21	8:H:29:VAL:HG11	1.97	0.46
2:M:228:GLU:HA	2:M:353:TYR:O	2.15	0.46
2:M:89:LEU:HD12	2:M:89:LEU:N	2.31	0.46
4:O:134:TYR:OH	4:O:156:PRO:HD3	2.16	0.46
11:V:93:LYS:HB3	11:V:93:LYS:NZ	2.30	0.46
1:A:283:GLN:NE2	1:A:373:GLN:NE2	2.63	0.46
4:D:113:ARG:NH1	24:D:5360:HOH:O	2.48	0.46
2:M:315:SER:O	2:M:318:ILE:HG22	2.15	0.46
1:A:156:HIS:HD2	1:A:159:ARG:NH2	2.13	0.46
3:C:57:ASN:HA	3:C:173:ASN:HD21	1.80	0.46
5:E:45:GLU:HB3	5:E:47:ASN:ND2	2.31	0.46
22:N:4131:CN3:HAA	7:R:85:HIS:CE1	2.51	0.46
21:O:4114:7PH:H25	21:O:4114:7PH:H2AA	1.97	0.46
3:C:142:TRP:CH2	5:P:165:VAL:HG23	2.51	0.46
10:U:61:ASN:HD22	10:U:62:PRO:N	2.13	0.46
20:C:4033:CN5:H2A	3:N:199:MET:HG2	1.97	0.46
8:S:35:LYS:O	8:S:37:LEU:N	2.49	0.45
2:B:44:LYS:HB2	2:B:47:VAL:CG2	2.47	0.45
5:E:55:TYR:O	5:E:59:MET:HG2	2.16	0.45
1:L:283:GLN:NE2	1:L:373:GLN:NE2	2.63	0.45
2:M:84:ARG:HD2	2:M:159:LEU:HD13	1.99	0.45
1:A:66:ASN:H	1:A:66:ASN:HD22	1.65	0.45
2:B:35:VAL:HG12	2:B:179:VAL:HG12	1.99	0.45
1:L:130:ASN:HD22	1:L:130:ASN:N	2.14	0.45
1:L:207:VAL:HG11	1:L:394:VAL:CG2	2.45	0.45
4:O:286:TRP:CZ3	5:P:56:ALA:HA	2.51	0.45
3:N:203:ILE:HB	8:S:8:THR:HG21	1.98	0.45
2:B:152:ARG:HD2	24:B:8523:HOH:O	2.17	0.45
2:B:68:VAL:O	2:B:72:GLU:HG3	2.17	0.45
3:C:32:MET:HE3	3:C:92:VAL:HG13	1.99	0.45
1:L:289:ASN:ND2	1:L:291:PHE:H	2.14	0.45
2:B:69:ARG:NH1	7:R:121:ASP:OD1	2.49	0.45
4:D:286:TRP:CD2	5:E:59:MET:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:HE2	2:B:263:ALA:HA	1.97	0.45
1:L:67:ASN:ND2	1:L:181:THR:HG23	2.31	0.45
1:L:47:HIS:CE1	2:M:22:ARG:HH22	2.35	0.45
2:M:146:LEU:HD13	2:M:354:VAL:HG22	1.99	0.45
10:U:21:THR:HG22	10:U:80:PHE:CD2	2.49	0.45
2:B:193:VAL:HG22	24:B:7468:HOH:O	2.15	0.45
2:M:71:SER:HA	2:M:74:LEU:HD12	1.99	0.45
10:U:37:TRP:CZ3	10:U:96:CYS:HB3	2.52	0.45
3:C:95:MET:HG2	18:C:4010:8PE:H37A	1.99	0.44
11:K:14:SER:HB2	11:K:17:ASP:OD2	2.17	0.44
2:M:74:LEU:HD13	2:M:101:TYR:OH	2.18	0.44
3:C:48:ILE:HD13	3:N:185:LEU:HG	1.98	0.44
3:N:18:ILE:HA	3:N:222:HIS:HB2	1.99	0.44
8:H:3:PRO:HG3	8:S:12:TRP:CE2	2.52	0.44
2:M:52:ASN:HD22	2:M:87:ILE:HG23	1.82	0.44
5:P:168:GLY:HA2	5:P:176:TRP:CD1	2.52	0.44
1:L:37:VAL:HG13	1:L:207:VAL:HA	2.00	0.44
2:M:44:LYS:HB2	2:M:47:VAL:CG2	2.47	0.44
3:N:216:LEU:HD12	3:N:216:LEU:N	2.33	0.44
15:A:4021:UMQ:O1'	9:I:18:VAL:HG13	2.17	0.44
7:G:18:SER:OG	7:G:21:LEU:HD23	2.17	0.44
1:L:57:SER:O	1:L:102:GLN:HB2	2.18	0.44
1:L:184:SER:O	1:L:188:LEU:HD13	2.17	0.44
1:A:60:ALA:O	1:A:173:PRO:HB3	2.17	0.44
1:A:39:ALA:HB1	1:A:390:LEU:HD11	1.99	0.44
2:B:318:ILE:HD13	2:B:343:VAL:HG22	1.99	0.44
5:E:208:ASP:O	5:E:211:LYS:HG2	2.17	0.44
7:R:80:GLN:O	7:R:84:THR:HG23	2.17	0.44
1:A:121:ASN:HD22	1:A:125:ILE:HD12	1.81	0.44
3:C:32:MET:CE	3:C:92:VAL:HG13	2.46	0.44
1:L:58:GLY:H	1:L:61:ASN:ND2	2.14	0.44
1:L:73:TRP:HA	1:L:76:ILE:HD11	1.99	0.44
2:B:66:LYS:O	2:B:70:GLU:HB2	2.18	0.44
10:J:21:THR:HG22	10:J:80:PHE:CD2	2.52	0.44
10:J:87:THR:HG22	10:J:88:THR:N	2.32	0.44
11:K:34:ASN:ND2	11:K:50:TYR:H	2.16	0.44
1:A:72:LEU:HD13	1:A:144:VAL:HG21	2.00	0.44
1:A:270:VAL:HG21	1:A:396:ILE:HD13	2.00	0.44
10:J:107:TYR:H	11:K:91:HIS:CD2	2.36	0.44
4:O:136:ASP:HB3	4:O:145:LYS:HG3	2.00	0.44
12:W:46:GLY:HA2	12:W:53:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:GLU:HG2	5:E:46:ASN:H	1.81	0.44
11:K:15:LEU:N	11:K:15:LEU:HD12	2.33	0.44
11:K:90:HIS:CD2	11:K:92:ILE:HG22	2.52	0.44
3:N:173:ASN:HB3	3:N:174:PRO:HD3	2.00	0.44
1:A:169:PHE:O	1:A:175:SER:HB3	2.18	0.43
1:A:380:SER:HB3	24:A:7013:HOH:O	2.17	0.43
1:A:69:VAL:HG23	1:A:193:LEU:HD22	2.00	0.43
10:J:40:LEU:HB3	10:J:93:THR:OG1	2.18	0.43
1:L:349:LYS:HE2	1:L:349:LYS:HA	2.00	0.43
4:O:286:TRP:CD2	5:P:59:MET:HG3	2.53	0.43
1:A:152:GLU:HG3	24:A:6944:HOH:O	2.18	0.43
1:A:172:THR:CG2	1:A:242:ALA:HA	2.48	0.43
11:K:34:ASN:ND2	11:K:49:TYR:HA	2.33	0.43
3:N:76:TYR:CG	4:O:262:GLU:HG3	2.53	0.43
5:E:106:ASN:ND2	5:E:119:ARG:HB2	2.33	0.43
8:H:35:LYS:O	8:H:37:LEU:N	2.46	0.43
11:V:6:GLN:HG2	11:V:23:CYS:SG	2.58	0.43
2:B:315:SER:HB2	2:B:316:PRO:HD3	2.00	0.43
2:B:62:ARG:HH21	2:B:62:ARG:CG	2.27	0.43
4:D:277:LEU:HD21	21:D:4014:7PH:H34	2.00	0.43
5:E:72:LYS:NZ	9:I:29:GLN:HE22	2.16	0.43
10:J:13:GLN:HA	10:J:121:SER:O	2.18	0.43
1:L:430:ASP:OD2	1:L:449:ARG:NH2	2.48	0.43
1:L:72:LEU:HD12	1:L:72:LEU:HA	1.88	0.43
2:M:124:LEU:HB3	2:M:128:ARG:NH2	2.33	0.43
7:G:120:LEU:HA	7:G:123:ILE:HG23	2.01	0.43
1:A:169:PHE:O	1:A:172:THR:HB	2.19	0.43
5:P:187:ILE:O	5:P:187:ILE:HG13	2.19	0.43
8:S:48:SER:O	8:S:49:PHE:HB2	2.18	0.43
11:V:27:GLN:HG2	11:V:28:ASP:N	2.34	0.43
12:W:65:ASP:H	12:W:68:ASN:ND2	2.14	0.43
1:A:38:VAL:HA	1:A:208:VAL:HG13	2.01	0.43
22:D:4031:CN3:HC	24:D:6590:HOH:O	2.19	0.43
1:L:227:ASN:N	1:L:227:ASN:HD22	2.17	0.43
1:L:252:ARG:HD2	8:S:21:GLN:HB2	2.00	0.43
12:W:10:LYS:HB2	12:W:10:LYS:NZ	2.33	0.43
3:C:362:TYR:O	3:C:367:VAL:HG23	2.19	0.43
4:D:123:GLU:H	4:D:123:GLU:CD	2.21	0.43
11:K:92:ILE:O	11:K:92:ILE:HD13	2.18	0.43
2:M:318:ILE:HG23	2:M:319:ASN:N	2.34	0.43
5:P:65:LEU:HD12	5:P:65:LEU:C	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:51:TYR:CD2	10:U:51:TYR:C	2.92	0.43
3:C:312:VAL:HG21	7:G:5:PHE:CZ	2.53	0.43
10:J:49:VAL:HG12	10:J:68:LEU:HD23	2.01	0.43
11:K:63:SER:HB2	11:K:74:THR:HB	2.01	0.43
1:L:62:GLU:OE1	1:L:67:ASN:HA	2.18	0.43
2:M:292:GLN:H	2:M:292:GLN:CD	2.22	0.43
3:N:58:ILE:HB	3:N:173:ASN:HA	2.01	0.43
8:S:47:ASN:O	8:S:50:ARG:HB3	2.19	0.43
2:B:146:LEU:HD12	2:B:146:LEU:HA	1.87	0.42
2:M:251:ALA:CB	2:M:339:ASN:HB2	2.49	0.42
10:U:38:ILE:CD1	10:U:46:LEU:HD22	2.49	0.42
3:C:216:LEU:HD12	3:C:216:LEU:N	2.34	0.42
5:E:103:LEU:O	5:E:120:HIS:O	2.37	0.42
8:H:41:PHE:O	8:H:42:HIS:HB3	2.19	0.42
2:M:317:ALA:O	2:M:321:THR:HG22	2.18	0.42
2:B:152:ARG:HG2	2:M:364:TYR:CZ	2.55	0.42
11:V:31:ASN:HD22	11:V:51:THR:HG21	1.84	0.42
3:C:173:ASN:HB3	3:C:174:PRO:HD3	2.01	0.42
3:C:25:SER:OG	7:G:79:HIS:HD2	2.02	0.42
1:L:127:GLN:HB3	1:L:130:ASN:ND2	2.34	0.42
5:P:203:PRO:O	5:P:205:TYR:HD1	2.02	0.42
11:V:2:ILE:N	11:V:2:ILE:HD12	2.29	0.42
2:B:35:VAL:HG12	2:B:179:VAL:CG1	2.50	0.42
1:L:349:LYS:HE2	1:L:352:ASN:OD1	2.20	0.42
2:M:40:ARG:HA	2:M:154:GLY:O	2.19	0.42
3:N:25:SER:OG	7:R:79:HIS:HD2	2.03	0.42
4:D:301:VAL:CG2	8:H:25:THR:HB	2.50	0.42
1:L:235:LYS:HB2	1:L:235:LYS:NZ	2.35	0.42
3:N:157:VAL:O	3:N:161:ILE:HG12	2.20	0.42
2:M:59:THR:HA	2:M:112:THR:HA	2.02	0.42
3:N:77:ILE:O	3:N:81:LEU:HB2	2.19	0.42
10:U:34:TYR:HB2	10:U:99:SER:OG	2.20	0.42
10:J:24:VAL:CG2	10:J:29:ILE:HD11	2.49	0.42
1:L:209:VAL:HG13	1:L:390:LEU:HD13	2.02	0.42
22:N:4131:CN3:CC	24:O:6998:HOH:O	2.68	0.42
7:R:45:PHE:O	7:R:48:LEU:HB2	2.19	0.42
10:U:98:ARG:O	10:U:109:MET:HA	2.19	0.42
10:U:48:TRP:CZ2	10:U:50:GLY:HA2	2.54	0.42
2:B:141:SER:HB2	24:B:7070:HOH:O	2.19	0.42
3:N:165:LEU:O	3:N:178:ARG:HD2	2.20	0.42
3:N:301:VAL:O	3:N:304:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:HG3	1:A:95:SER:HB3	2.01	0.41
2:B:362:LEU:HD12	2:B:362:LEU:HA	1.90	0.41
11:K:4:LEU:N	11:K:4:LEU:HD12	2.34	0.41
5:P:85:THR:O	5:P:88:VAL:HG22	2.20	0.41
1:A:169:PHE:HB3	1:A:172:THR:HG22	2.02	0.41
1:A:145:LEU:HD11	1:A:185:LEU:HB3	2.01	0.41
1:A:57:SER:O	1:A:102:GLN:HB2	2.20	0.41
2:B:230:ARG:NE	2:B:359:VAL:HG13	2.34	0.41
2:B:255:VAL:HG23	2:B:314:LEU:HD13	2.02	0.41
2:M:98:LEU:N	2:M:99:PRO:HD2	2.35	0.41
4:O:296:LYS:HE3	24:O:5628:HOH:O	2.19	0.41
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.85	0.41
14:A:4013:6PH:H38	3:C:230:LEU:HD11	2.02	0.41
3:C:121:PHE:CZ	3:C:125:ILE:HD11	2.55	0.41
11:K:34:ASN:ND2	11:K:91:HIS:HE1	2.18	0.41
2:M:112:THR:OG1	2:M:114:PHE:CE2	2.74	0.41
3:N:20:SER:HA	3:N:21:PRO:HD3	1.93	0.41
10:U:18:LEU:O	10:U:82:LYS:HA	2.20	0.41
11:V:15:LEU:N	11:V:15:LEU:HD12	2.34	0.41
11:V:32:PHE:HB2	11:V:92:ILE:HG22	2.03	0.41
3:C:117:GLY:O	16:C:4002:HEM:HMC3	2.21	0.41
3:C:214:GLY:O	3:C:218:ARG:CD	2.69	0.41
1:L:115:LYS:HD2	1:L:115:LYS:HA	1.88	0.41
2:M:254:GLU:HG2	2:M:276:LEU:HD23	2.02	0.41
3:N:48:ILE:HD12	3:N:184:TYR:OH	2.21	0.41
7:R:18:SER:OG	7:R:21:LEU:HD23	2.20	0.41
8:S:48:SER:C	8:S:50:ARG:H	2.23	0.41
11:V:21:ILE:HG22	11:V:22:SER:N	2.35	0.41
11:V:53:ARG:NH2	11:V:53:ARG:HG3	2.35	0.41
1:A:172:THR:HG23	1:A:242:ALA:HA	2.03	0.41
10:J:76:LYS:HB2	10:J:78:GLN:HG2	2.02	0.41
1:L:241:LYS:HD2	1:L:241:LYS:N	2.35	0.41
2:M:312:LYS:HB3	2:M:312:LYS:HE2	1.75	0.41
2:M:230:ARG:NE	2:M:359:VAL:HG13	2.35	0.41
3:N:166:TRP:CE3	3:N:170:SER:HA	2.54	0.41
2:B:230:ARG:HE	2:B:359:VAL:HG13	1.85	0.41
5:E:165:VAL:HG23	3:N:142:TRP:CH2	2.56	0.41
1:L:289:ASN:HD22	1:L:291:PHE:H	1.69	0.41
1:L:74:LYS:HG3	1:L:95:SER:HB3	2.01	0.41
1:A:364:GLU:HG3	7:R:125:VAL:HG21	2.03	0.41
2:B:193:VAL:O	2:B:193:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:ILE:HD12	17:C:4005:SMA:H14	2.02	0.41
11:K:48:ILE:HD13	11:K:54:LEU:HA	2.03	0.41
1:L:424:LYS:HD2	1:L:424:LYS:HA	1.94	0.41
4:O:111:ALA:HA	4:O:154:TYR:HA	2.02	0.41
8:S:49:PHE:O	8:S:53:LYS:HB2	2.21	0.41
8:H:2:GLY:HA2	8:H:3:PRO:HD3	1.83	0.41
7:R:91:ASN:HD22	7:R:91:ASN:H	1.69	0.41
11:V:2:ILE:H	11:V:2:ILE:CD1	2.32	0.41
2:B:336:ILE:HD12	2:B:336:ILE:N	2.35	0.40
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.60	0.40
2:M:197:LEU:O	2:M:201:VAL:HG23	2.20	0.40
1:A:179:ARG:NH2	1:A:179:ARG:CG	2.81	0.40
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.35	0.40
1:A:228:LEU:HG	1:A:229:SER:N	2.36	0.40
2:M:50:LEU:HA	2:M:50:LEU:HD23	1.92	0.40
16:N:4021:HEM:HBC2	16:N:4021:HEM:HHD	2.02	0.40
2:B:112:THR:OG1	2:B:114:PHE:CE2	2.74	0.40
2:B:146:LEU:HG	2:B:242:GLY:HA3	2.03	0.40
2:B:164:VAL:CG2	2:M:232:ARG:NH1	2.84	0.40
10:J:40:LEU:HB3	10:J:93:THR:HG1	1.87	0.40
3:C:104:GLY:HA2	3:C:106:TYR:CE2	2.56	0.40
2:B:181:THR:HB	2:B:212:GLY:H	1.86	0.40
5:E:106:ASN:HD21	5:E:119:ARG:HD2	1.86	0.40
1:L:228:LEU:O	1:L:228:LEU:HD12	2.22	0.40
1:L:43:ASN:HA	1:L:44:PRO:HD2	1.92	0.40
2:M:137:CYS:HA	2:M:138:PRO:HD2	1.93	0.40
7:R:100:VAL:HG13	7:R:101:PRO:HD2	2.02	0.40
8:S:7:LYS:HD3	8:S:7:LYS:HA	1.84	0.40
11:V:33:LEU:HD13	11:V:71:TYR:CD1	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	408 (95%)	19 (4%)	2 (0%)	29	18
1	L	429/431 (100%)	406 (95%)	19 (4%)	4 (1%)	17	7
2	B	350/352 (99%)	330 (94%)	15 (4%)	5 (1%)	11	3
2	M	350/352 (99%)	330 (94%)	19 (5%)	1 (0%)	41	31
3	C	383/385 (100%)	370 (97%)	12 (3%)	1 (0%)	41	31
3	N	383/385 (100%)	369 (96%)	13 (3%)	1 (0%)	41	31
4	D	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
4	O	246/248 (99%)	241 (98%)	4 (2%)	1 (0%)	34	24
5	E	183/185 (99%)	173 (94%)	8 (4%)	2 (1%)	14	5
5	P	183/185 (99%)	169 (92%)	10 (6%)	4 (2%)	6	1
6	F	72/146 (49%)	71 (99%)	1 (1%)	0	100	100
6	Q	72/146 (49%)	70 (97%)	2 (3%)	0	100	100
7	G	124/126 (98%)	122 (98%)	2 (2%)	0	100	100
7	R	124/126 (98%)	123 (99%)	1 (1%)	0	100	100
8	H	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	14	5
8	S	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	14	5
9	I	55/65 (85%)	53 (96%)	2 (4%)	0	100	100
9	T	55/65 (85%)	52 (94%)	2 (4%)	1 (2%)	8	2
10	J	125/127 (98%)	114 (91%)	11 (9%)	0	100	100
10	U	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
11	K	105/107 (98%)	91 (87%)	10 (10%)	4 (4%)	3	0
11	V	105/107 (98%)	91 (87%)	11 (10%)	3 (3%)	4	1
12	W	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
All	All	4432/4638 (96%)	4206 (95%)	195 (4%)	31 (1%)	22	12

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	103	LEU
5	P	103	LEU
2	B	153	LYS
3	C	223	SER
1	L	228	LEU
3	N	223	SER
11	V	30	ASN

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Mol	Chain	Res	Type
1	A	128	LYS
2	B	335	PRO
11	K	51	THR
1	L	232	THR
2	M	342	ALA
4	O	308	ARG
8	S	36	PRO
9	T	13	ARG
2	B	337	GLU
8	H	36	PRO
1	L	34	ASN
5	P	209	GLY
1	A	29	VAL
2	B	332	VAL
2	B	339	ASN
5	E	46	ASN
1	L	227	ASN
5	P	47	ASN
5	P	102	PRO
11	V	51	THR
11	K	68	GLY
11	V	16	GLY
11	K	9	VAL
11	K	80	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	343 (93%)	27 (7%)	14	6
1	L	370/370 (100%)	340 (92%)	30 (8%)	11	4
2	B	301/301 (100%)	288 (96%)	13 (4%)	29	19
2	M	301/301 (100%)	282 (94%)	19 (6%)	18	8
3	C	338/338 (100%)	318 (94%)	20 (6%)	19	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	338/338 (100%)	321 (95%)	17 (5%)	24	15
4	D	206/206 (100%)	200 (97%)	6 (3%)	42	35
4	O	206/206 (100%)	202 (98%)	4 (2%)	57	53
5	E	151/151 (100%)	149 (99%)	2 (1%)	69	68
5	P	151/151 (100%)	146 (97%)	5 (3%)	38	29
6	F	67/130 (52%)	62 (92%)	5 (8%)	13	5
6	Q	67/130 (52%)	63 (94%)	4 (6%)	19	9
7	G	110/110 (100%)	105 (96%)	5 (4%)	27	18
7	R	110/110 (100%)	107 (97%)	3 (3%)	44	38
8	H	77/77 (100%)	74 (96%)	3 (4%)	32	23
8	S	77/77 (100%)	76 (99%)	1 (1%)	69	68
9	I	47/53 (89%)	46 (98%)	1 (2%)	53	48
9	T	47/53 (89%)	45 (96%)	2 (4%)	29	19
10	J	112/112 (100%)	105 (94%)	7 (6%)	18	8
10	U	112/112 (100%)	107 (96%)	5 (4%)	27	18
11	K	93/93 (100%)	88 (95%)	5 (5%)	22	13
11	V	93/93 (100%)	90 (97%)	3 (3%)	39	30
12	W	89/88 (101%)	87 (98%)	2 (2%)	52	47
All	All	3833/3970 (96%)	3644 (95%)	189 (5%)	25	15

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	66	ASN
1	A	120	LEU
1	A	126	GLN
1	A	145	LEU
1	A	164	LEU
1	A	172	THR
1	A	179	ARG
1	A	185	LEU
1	A	188	LEU
1	A	193	LEU
1	A	239	LYS
1	A	240	LYS

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Mol	Chain	Res	Type
1	A	241	LYS
1	A	252	ARG
1	A	289	ASN
1	A	311	LEU
1	A	320	LEU
1	A	330	PHE
1	A	336	ASN
1	A	343	LEU
1	A	360	ASP
1	A	370	LEU
1	A	374	LEU
1	A	425	ARG
1	A	426	LEU
1	A	443	LEU
2	B	53	ARG
2	B	54	PHE
2	B	73	LEU
2	B	84	ARG
2	B	128	ARG
2	B	144	ASP
2	B	146	LEU
2	B	169	LEU
2	B	254	GLU
2	B	312	LYS
2	B	345	ASP
2	B	347	LYS
2	B	362	LEU
3	C	10	LEU
3	C	35	LEU
3	C	38	LEU
3	C	60	LEU
3	C	79	ARG
3	C	81	LEU
3	C	89	PHE
3	C	99	LYS
3	C	150	LEU
3	C	182	LEU
3	C	184	TYR
3	C	185	LEU
3	C	238	LEU
3	C	302	LEU
3	C	313	VAL

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Mol	Chain	Res	Type
3	C	336	LEU
3	C	347	PRO
3	C	350	LEU
3	C	377	LEU
3	C	382	ARG
4	D	69	LEU
4	D	113	ARG
4	D	251	VAL
4	D	256	ASN
4	D	280	LEU
4	D	283	LEU
5	E	65	LEU
5	E	114	LYS
6	F	77	GLN
6	F	89	GLU
6	F	94	LEU
6	F	130	LEU
6	F	131	GLN
7	G	16	LEU
7	G	31	GLN
7	G	91	ASN
7	G	97	GLN
7	G	127	LYS
8	H	56	PHE
8	H	60	LEU
8	H	89	LEU
9	I	55	ARG
10	J	38	ILE
10	J	39	ARG
10	J	51	TYR
10	J	59	ASN
10	J	61	ASN
10	J	68	LEU
10	J	114	GLN
11	K	30	ASN
11	K	38	GLN
11	K	81	GLU
11	K	92	ILE
11	K	93	LYS
1	L	66	ASN
1	L	76	ILE
1	L	120	LEU

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Mol	Chain	Res	Type
1	L	150	ASP
1	L	152	GLU
1	L	164	LEU
1	L	172	THR
1	L	174	LEU
1	L	176	LEU
1	L	179	ARG
1	L	185	LEU
1	L	188	LEU
1	L	213	ASN
1	L	227	ASN
1	L	241	LYS
1	L	252	ARG
1	L	261	ILE
1	L	271	ASN
1	L	289	ASN
1	L	311	LEU
1	L	320	LEU
1	L	330	PHE
1	L	336	ASN
1	L	343	LEU
1	L	370	LEU
1	L	373	GLN
1	L	374	LEU
1	L	390	LEU
1	L	425	ARG
1	L	443	LEU
2	M	17	LEU
2	M	53	ARG
2	M	54	PHE
2	M	73	LEU
2	M	74	LEU
2	M	84	ARG
2	M	144	ASP
2	M	146	LEU
2	M	169	LEU
2	M	190	GLU
2	M	206	LEU
2	M	218	LYS
2	M	246	ASN
2	M	250	LEU
2	M	254	GLU

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Mol	Chain	Res	Type
2	M	292	GLN
2	M	312	LYS
2	M	330	GLU
2	M	362	LEU
3	N	35	LEU
3	N	38	LEU
3	N	79	ARG
3	N	89	PHE
3	N	99	LYS
3	N	109	PRO
3	N	150	LEU
3	N	182	LEU
3	N	184	TYR
3	N	185	LEU
3	N	208	ASN
3	N	238	LEU
3	N	312	VAL
3	N	336	LEU
3	N	350	LEU
3	N	377	LEU
3	N	382	ARG
4	O	69	LEU
4	O	256	ASN
4	O	280	LEU
4	O	283	LEU
5	P	41	ASP
5	P	44	LYS
5	P	45	GLU
5	P	65	LEU
5	P	211	LYS
6	Q	77	GLN
6	Q	94	LEU
6	Q	103	GLU
6	Q	111	GLN
7	R	2	PRO
7	R	16	LEU
7	R	41	LEU
8	S	87	GLU
9	T	18	VAL
9	T	55	ARG
10	U	39	ARG
10	U	51	TYR

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Mol	Chain	Res	Type
10	U	61	ASN
10	U	68	LEU
10	U	114	GLN
11	V	18	ARG
11	V	92	ILE
11	V	93	LYS
12	W	68	ASN
12	W	75	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	66	ASN
1	A	67	ASN
1	A	102	GLN
1	A	121	ASN
1	A	126	GLN
1	A	156	HIS
1	A	199	ASN
1	A	213	ASN
1	A	283	GLN
1	A	289	ASN
1	A	317	HIS
1	A	336	ASN
1	A	350	GLN
1	A	373	GLN
1	A	388	ASN
1	A	429	GLN
2	B	49	HIS
2	B	52	ASN
2	B	55	ASN
2	B	258	ASN
2	B	339	ASN
3	C	14	ASN
3	C	22	GLN
3	C	74	ASN
3	C	173	ASN
3	C	204	HIS
3	C	208	ASN
3	C	253	HIS
3	C	332	ASN

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Mol	Chain	Res	Type
4	D	78	HIS
4	D	79	ASN
4	D	127	ASN
5	E	38	ASN
5	E	47	ASN
5	E	106	ASN
5	E	184	HIS
6	F	77	GLN
6	F	109	GLN
6	F	110	GLN
7	G	31	GLN
7	G	53	ASN
7	G	57	GLN
7	G	79	HIS
7	G	91	ASN
7	G	97	GLN
8	H	74	ASN
9	I	14	ASN
9	I	29	GLN
10	J	59	ASN
10	J	61	ASN
10	J	77	ASN
10	J	78	GLN
10	J	114	GLN
11	K	27	GLN
11	K	30	ASN
11	K	31	ASN
11	K	34	ASN
11	K	38	GLN
11	K	89	GLN
11	K	90	HIS
11	K	91	HIS
1	L	31	GLN
1	L	47	HIS
1	L	61	ASN
1	L	66	ASN
1	L	67	ASN
1	L	102	GLN
1	L	122	GLN
1	L	127	GLN
1	L	130	ASN
1	L	136	ASN

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Mol	Chain	Res	Type
1	L	156	HIS
1	L	170	GLN
1	L	213	ASN
1	L	227	ASN
1	L	271	ASN
1	L	283	GLN
1	L	289	ASN
1	L	317	HIS
1	L	336	ASN
1	L	350	GLN
1	L	385	ASN
1	L	388	ASN
1	L	438	GLN
2	M	49	HIS
2	M	52	ASN
2	M	55	ASN
2	M	246	ASN
2	M	252	GLN
2	M	292	GLN
3	N	14	ASN
3	N	43	GLN
3	N	74	ASN
3	N	173	ASN
3	N	208	ASN
3	N	253	HIS
3	N	332	ASN
4	O	78	HIS
4	O	79	ASN
4	O	127	ASN
4	O	170	GLN
4	O	303	ASN
5	P	97	ASN
5	P	106	ASN
5	P	184	HIS
6	Q	77	GLN
6	Q	109	GLN
6	Q	119	HIS
7	R	30	ASN
7	R	53	ASN
7	R	57	GLN
7	R	79	HIS
7	R	91	ASN

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Mol	Chain	Res	Type
8	S	55	GLN
8	S	74	ASN
9	T	14	ASN
9	T	29	GLN
10	U	61	ASN
10	U	77	ASN
10	U	78	GLN
10	U	114	GLN
11	V	31	ASN
11	V	34	ASN
11	V	38	GLN
11	V	89	GLN
11	V	90	HIS
11	V	91	HIS
12	W	67	ASN
12	W	68	ASN
12	W	75	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
12	M3L	W	77	12	10,11,12	0.89	0	9,14,16	0.99	1 (11%)

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
12	M3L	W	77	12	-	0/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	W	77	M3L	CM2-NZ-CM1	-2.07	103.64	108.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

2 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	$\# Z  > 2$
13	GLC	X	1	13	11,11,12	0.64	0	15,15,17	0.81	1 (6%)
13	FRU	X	2	13	11,12,12	0.56	0	10,18,18	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GLC	X	1	13	-	2/2/19/22	0/1/1/1
13	FRU	X	2	13	-	0/5/24/24	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X	1	GLC	C2-C3-C4	-2.88	105.92	110.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

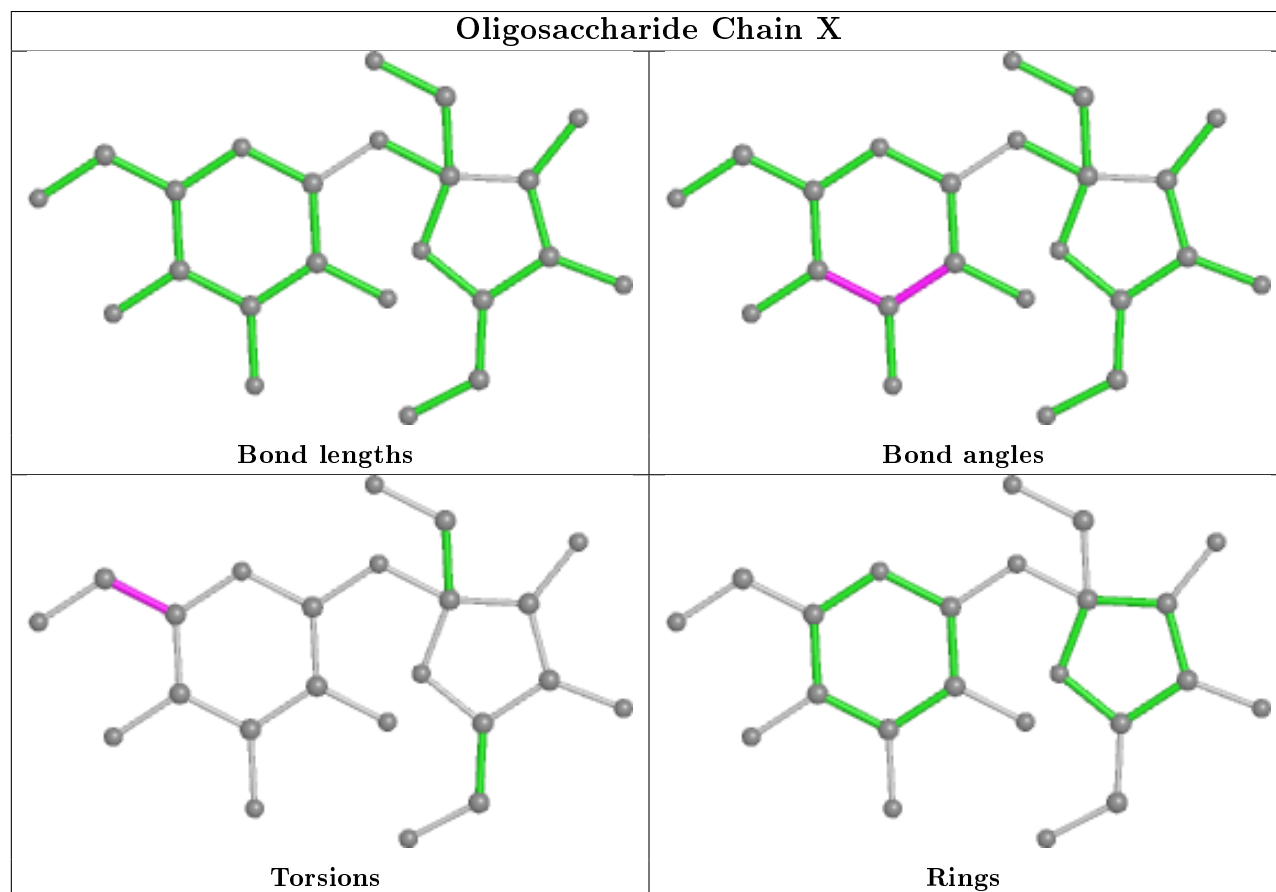
Mol	Chain	Res	Type	Atoms
13	X	1	GLC	C4-C5-C6-O6
13	X	1	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	X	1	GLC	1	0
13	X	2	FRU	4	0

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



## 5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	9PE	N	4111	-	39,39,39	0.73	0	42,44,44	0.99	1 (2%)
16	HEM	N	4022	3	27,50,50	1.67	8 (29%)	17,82,82	1.16	2 (11%)
21	7PH	D	4014	-	37,37,37	0.97	1 (2%)	41,42,42	1.55	9 (21%)
23	FES	E	4004	5	0,4,4	0.00	-	-		
22	CN3	D	4031	-	54,54,54	1.51	9 (16%)	60,66,66	1.49	8 (13%)
14	6PH	A	4013	-	39,39,39	0.97	2 (5%)	43,44,44	1.46	5 (11%)
22	CN3	N	4131	-	54,54,54	1.49	10 (18%)	60,66,66	1.47	7 (11%)
16	HEM	O	4023	4	27,50,50	1.77	6 (22%)	17,82,82	1.20	1 (5%)
23	FES	P	4024	5	0,4,4	0.00	-	-		
15	UMQ	A	4021	-	35,35,35	0.92	1 (2%)	46,46,46	1.80	7 (15%)
20	CN5	C	4033	-	40,40,40	1.64	11 (27%)	44,48,48	1.87	9 (20%)
14	6PH	L	4113	-	39,39,39	0.98	2 (5%)	43,44,44	1.51	5 (11%)
16	HEM	C	4001	3	27,50,50	1.72	5 (18%)	17,82,82	0.97	1 (5%)
16	HEM	C	4002	3	27,50,50	1.65	7 (25%)	17,82,82	1.23	2 (11%)
17	SMA	C	4005	-	35,38,38	0.90	2 (5%)	46,52,52	1.62	6 (13%)
17	SMA	N	4025	-	35,38,38	0.90	2 (5%)	46,52,52	1.71	8 (17%)
18	8PE	N	4110	-	46,46,46	0.98	3 (6%)	49,51,51	1.13	2 (4%)
16	HEM	W	4026	12	27,50,50	1.65	5 (18%)	17,82,82	1.13	1 (5%)
15	UMQ	L	4121	-	35,35,35	0.96	1 (2%)	46,46,46	1.77	5 (10%)
18	8PE	C	4010	-	46,46,46	0.95	2 (4%)	49,51,51	1.17	2 (4%)
21	7PH	O	4114	-	37,37,37	0.97	2 (5%)	41,42,42	1.56	9 (21%)
19	9PE	C	4011	-	39,39,39	0.69	0	42,44,44	0.96	1 (2%)
16	HEM	N	4021	3	27,50,50	1.79	6 (22%)	17,82,82	1.01	1 (5%)
16	HEM	D	4003	4	27,50,50	1.68	6 (22%)	17,82,82	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	9PE	N	4111	-	-	18/43/43/43	-
16	HEM	N	4022	3	-	0/6/54/54	-
21	7PH	D	4014	-	-	13/39/39/39	-
23	FES	E	4004	5	-	-	0/1/1/1
22	CN3	D	4031	-	-	32/65/65/65	-
14	6PH	A	4013	-	-	18/41/41/41	-
22	CN3	N	4131	-	-	32/65/65/65	-
16	HEM	O	4023	4	-	0/6/54/54	-
23	FES	P	4024	5	-	-	0/1/1/1
15	UMQ	A	4021	-	-	4/20/60/60	0/2/2/2
20	CN5	C	4033	-	-	19/44/44/44	-
14	6PH	L	4113	-	-	19/41/41/41	-
16	HEM	C	4001	3	-	0/6/54/54	-
16	HEM	C	4002	3	-	0/6/54/54	-
17	SMA	C	4005	-	-	3/33/34/34	0/2/2/2
17	SMA	N	4025	-	-	0/33/34/34	0/2/2/2
18	8PE	N	4110	-	-	22/50/50/50	-
16	HEM	W	4026	12	-	0/6/54/54	-
16	HEM	N	4021	3	-	0/6/54/54	-
18	8PE	C	4010	-	-	19/50/50/50	-
21	7PH	O	4114	-	-	12/39/39/39	-
19	9PE	C	4011	-	-	21/43/43/43	-
15	UMQ	L	4121	-	-	4/20/60/60	0/2/2/2
16	HEM	D	4003	4	-	0/6/54/54	-

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	4031	CN3	O31-C3	-4.31	1.35	1.45
22	N	4131	CN3	O31-C3	-4.29	1.35	1.45
16	C	4001	HEM	C3C-CAC	-4.10	1.39	1.47
16	N	4021	HEM	C3C-CAC	-4.06	1.39	1.47
16	N	4021	HEM	C3B-CAB	-3.81	1.40	1.47
16	C	4001	HEM	C3B-CAB	-3.80	1.40	1.47
16	N	4021	HEM	C3C-C2C	-3.79	1.35	1.40
16	O	4023	HEM	C3B-C2B	-3.79	1.35	1.40
16	D	4003	HEM	C3B-C2B	-3.79	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	4003	HEM	CBC-CAC	3.78	1.54	1.29
16	O	4023	HEM	CBC-CAC	3.78	1.54	1.29
16	O	4023	HEM	CBB-CAB	3.72	1.54	1.29
20	C	4033	CN5	P-O14	3.70	1.64	1.50
16	W	4026	HEM	CBC-CAC	3.66	1.53	1.29
16	D	4003	HEM	CBB-CAB	3.64	1.53	1.29
22	D	4031	CN3	O3'-CA	-3.57	1.31	1.44
16	W	4026	HEM	CBB-CAB	3.55	1.52	1.29
21	D	4014	7PH	O31-C3	-3.54	1.37	1.45
16	C	4001	HEM	C3C-C2C	-3.53	1.35	1.40
22	D	4031	CN3	O21-C2	-3.50	1.37	1.46
22	N	4131	CN3	O3'-CA	-3.49	1.31	1.44
15	A	4021	UMQ	C3-C2	-3.44	1.43	1.52
20	C	4033	CN5	O3'-CA	-3.43	1.31	1.44
21	O	4114	7PH	O31-C3	-3.43	1.37	1.45
15	L	4121	UMQ	C3-C2	-3.42	1.43	1.52
18	C	4010	8PE	O21-C21	3.41	1.43	1.34
16	W	4026	HEM	C3B-C2B	-3.40	1.35	1.40
16	D	4003	HEM	C3C-C2C	-3.39	1.35	1.40
16	N	4022	HEM	C3C-C2C	-3.37	1.35	1.40
16	N	4022	HEM	C3B-CAB	-3.37	1.41	1.47
22	N	4131	CN3	O21-C2	-3.35	1.38	1.46
18	N	4110	8PE	O21-C21	3.32	1.43	1.34
16	C	4002	HEM	C3B-C2B	-3.30	1.35	1.40
16	O	4023	HEM	C3C-C2C	-3.24	1.35	1.40
16	N	4022	HEM	C3B-C2B	-3.23	1.35	1.40
16	O	4023	HEM	C3B-CAB	3.21	1.54	1.47
16	N	4021	HEM	C3B-C2B	-3.19	1.35	1.40
16	W	4026	HEM	C3C-C2C	-3.18	1.36	1.40
16	C	4002	HEM	C3C-C2C	-3.15	1.36	1.40
16	C	4001	HEM	C3B-C2B	-3.10	1.36	1.40
20	C	4033	CN5	P'-O2'	3.02	1.61	1.50
16	W	4026	HEM	C3B-CAB	2.98	1.54	1.47
16	C	4002	HEM	C3B-CAB	-2.97	1.41	1.47
16	N	4022	HEM	C3C-CAC	-2.95	1.41	1.47
16	D	4003	HEM	C3B-CAB	2.90	1.53	1.47
16	O	4023	HEM	C3C-CAC	2.89	1.53	1.47
16	C	4002	HEM	CBB-CAB	2.86	1.48	1.29
20	C	4033	CN5	P-O11	2.82	1.70	1.59
20	C	4033	CN5	OA-CB	2.81	1.51	1.43
16	C	4002	HEM	C3C-CAC	-2.79	1.42	1.47
22	N	4131	CN3	O32-C31	-2.77	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	4031	CN3	O11-C1	-2.64	1.34	1.44
17	N	4025	SMA	O1-C2	2.61	1.38	1.35
20	C	4033	CN5	CC-CB	2.59	1.60	1.51
22	N	4131	CN3	O21-C21	2.55	1.41	1.34
22	D	4031	CN3	O32-C31	-2.54	1.15	1.22
22	D	4031	CN3	CC-CB	2.50	1.60	1.51
22	D	4031	CN3	O21-C21	2.50	1.41	1.34
16	C	4002	HEM	CMA-C3A	2.50	1.56	1.51
14	L	4113	6PH	C1-C2	2.47	1.58	1.50
22	N	4131	CN3	O11-C1	-2.47	1.35	1.44
22	N	4131	CN3	CA-CB	2.46	1.59	1.51
16	N	4022	HEM	CBB-CAB	2.45	1.45	1.29
22	N	4131	CN3	CC-CB	2.43	1.59	1.51
16	N	4022	HEM	CMC-C2C	2.42	1.57	1.51
17	N	4025	SMA	C4-C3	2.40	1.48	1.41
14	L	4113	6PH	C3-C2	2.39	1.58	1.50
22	D	4031	CN3	CA-CB	2.36	1.59	1.51
18	N	4110	8PE	O32-C31	-2.34	1.15	1.22
17	C	4005	SMA	O1-C2	2.33	1.38	1.35
16	C	4002	HEM	CBC-CAC	2.33	1.44	1.29
14	A	4013	6PH	C1-C2	2.32	1.57	1.50
22	D	4031	CN3	OA-CB	2.26	1.50	1.43
17	C	4005	SMA	C4-C3	2.26	1.47	1.41
14	A	4013	6PH	C3-C2	2.24	1.57	1.50
22	N	4131	CN3	O41-C3'	-2.23	1.40	1.45
18	C	4010	8PE	O32-C31	-2.23	1.15	1.22
16	N	4021	HEM	CBB-CAB	2.22	1.43	1.29
18	N	4110	8PE	C1-C2	2.20	1.57	1.50
22	N	4131	CN3	OA-CB	2.18	1.49	1.43
16	C	4001	HEM	CBC-CAC	2.17	1.43	1.29
16	N	4022	HEM	CMA-C3A	2.16	1.56	1.51
16	N	4022	HEM	CBC-CAC	2.15	1.43	1.29
16	N	4021	HEM	CBC-CAC	2.14	1.43	1.29
20	C	4033	CN5	P'-O1'	2.13	1.67	1.59
20	C	4033	CN5	C42-C41	2.07	1.56	1.49
20	C	4033	CN5	O31-C3	-2.04	1.39	1.45
20	C	4033	CN5	C2'-C3'	-2.04	1.42	1.51
16	D	4003	HEM	C3C-CAC	2.03	1.52	1.47
20	C	4033	CN5	P'-O4'	2.02	1.64	1.55
21	O	4114	7PH	O22-C21	-2.01	1.16	1.22

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	4021	UMQ	CA-O1'-C1'	-8.98	98.95	113.84
15	L	4121	UMQ	CA-O1'-C1'	-8.69	99.44	113.84
20	C	4033	CN5	O1'-C1'-C2'	6.39	130.30	108.99
17	C	4005	SMA	C3-C4-C4A	-5.94	114.60	120.58
17	N	4025	SMA	C3-C4-C4A	-5.78	114.77	120.58
22	D	4031	CN3	C2'-O51-C51	-5.18	105.03	117.79
17	N	4025	SMA	C9-C2-C3	5.12	127.65	120.39
14	L	4113	6PH	P-O11-C1	5.10	132.33	118.30
22	N	4131	CN3	C2'-O51-C51	-4.95	105.60	117.79
20	C	4033	CN5	C3'-C2'-C1'	-4.82	97.68	113.70
14	A	4013	6PH	P-O11-C1	4.78	131.45	118.30
17	C	4005	SMA	C9-C2-C3	4.54	126.83	120.39
21	O	4114	7PH	P-O11-C1	4.28	130.09	118.30
21	D	4014	7PH	P-O11-C1	4.19	129.83	118.30
20	C	4033	CN5	P'-O1'-C1'	-4.19	100.98	121.59
20	C	4033	CN5	O11-C1-C2	-4.03	95.52	108.99
14	L	4113	6PH	C3-C2-C1	-4.01	102.31	111.79
14	A	4013	6PH	C3-C2-C1	-3.99	102.36	111.79
17	N	4025	SMA	C4-C3-C2	3.84	120.84	116.63
17	C	4005	SMA	C4-C3-C2	3.81	120.81	116.63
17	N	4025	SMA	C9-C10-C11	-3.79	109.61	114.72
19	N	4111	9PE	C2-O21-C21	-3.79	108.47	117.79
22	N	4131	CN3	C2-O21-C21	-3.78	108.50	117.79
15	L	4121	UMQ	O1'-CA-CB	3.75	122.69	109.56
16	C	4002	HEM	CMC-C2C-C3C	3.62	131.46	124.68
21	D	4014	7PH	C38-C37-C36	-3.62	96.04	114.42
22	D	4031	CN3	C2-O21-C21	-3.62	108.89	117.79
21	O	4114	7PH	C38-C37-C36	-3.58	96.23	114.42
16	N	4022	HEM	CMC-C2C-C3C	3.57	131.36	124.68
19	C	4011	9PE	C2-O21-C21	-3.55	109.04	117.79
22	D	4031	CN3	C3-C2-C1	-3.53	103.44	111.79
15	A	4021	UMQ	O1'-CA-CB	3.52	121.89	109.56
18	C	4010	8PE	C3-C2-C1	3.47	119.99	111.79
18	C	4010	8PE	C2-O21-C21	-3.45	109.29	117.79
14	A	4013	6PH	O11-P-O12	3.40	116.01	106.47
21	O	4114	7PH	O12-P-O11	3.39	115.75	106.73
22	N	4131	CN3	C3-C2-C1	-3.39	103.77	111.79
21	D	4014	7PH	O12-P-O11	3.36	115.68	106.73
14	L	4113	6PH	O11-P-O12	3.36	115.89	106.47
18	N	4110	8PE	C2-O21-C21	-3.35	109.54	117.79
17	C	4005	SMA	C9-C10-C11	-3.20	110.41	114.72
14	L	4113	6PH	O13-P-O11	3.14	115.10	106.73
18	N	4110	8PE	C3-C2-C1	3.11	119.14	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	4031	CN3	P-O13-CC	3.09	139.82	121.68
14	A	4013	6PH	O13-P-O11	2.98	114.67	106.73
21	D	4014	7PH	C3-C2-C1	-2.98	104.74	111.79
22	N	4131	CN3	P-O13-CC	2.97	139.12	121.68
22	D	4031	CN3	C3'-C2'-C1'	-2.97	104.75	111.79
21	D	4014	7PH	O13-P-O11	2.89	114.42	106.73
21	O	4114	7PH	O13-P-O11	2.87	114.36	106.73
21	O	4114	7PH	C3-C2-C1	-2.86	105.03	111.79
20	C	4033	CN5	P-O13-CC	2.69	137.44	121.68
22	N	4131	CN3	P-O11-C1	-2.65	106.11	121.68
14	L	4113	6PH	O14-P-O11	-2.61	99.78	106.73
22	D	4031	CN3	P-O11-C1	-2.61	106.39	121.68
17	N	4025	SMA	O1-C2-C9	-2.58	108.84	111.91
22	N	4131	CN3	O4'-P'-O3'	2.57	119.69	107.75
16	N	4021	HEM	CBA-CAA-C2A	-2.56	107.77	112.49
16	C	4002	HEM	CMB-C2B-C3B	2.55	129.45	124.68
15	A	4021	UMQ	CD-CC-CB	-2.49	101.79	114.42
20	C	4033	CN5	C33-C32-C31	2.47	122.59	113.62
16	O	4023	HEM	CMD-C2D-C1D	-2.45	124.70	128.46
22	N	4131	CN3	C3'-C2'-C1'	-2.44	106.02	111.79
15	L	4121	UMQ	C3'-C4'-C5'	-2.43	105.37	110.93
14	A	4013	6PH	O14-P-O11	-2.42	100.29	106.73
21	D	4014	7PH	O11-P-O14	-2.39	99.76	106.47
15	L	4121	UMQ	CD-CC-CB	-2.39	102.29	114.42
20	C	4033	CN5	C3-C2-C1	-2.39	105.76	113.70
22	D	4031	CN3	O4'-P'-O3'	2.38	118.79	107.75
16	N	4022	HEM	CMB-C2B-C3B	2.33	129.04	124.68
15	A	4021	UMQ	C3'-C4'-C5'	-2.33	105.59	110.93
15	A	4021	UMQ	O1-C1-O5	-2.29	104.27	110.67
21	O	4114	7PH	O31-C3-C2	-2.28	101.79	108.43
17	N	4025	SMA	O1-C8A-C4A	2.28	123.21	120.87
21	O	4114	7PH	O11-P-O14	-2.26	100.14	106.47
21	O	4114	7PH	O31-C31-C32	-2.25	104.84	111.91
17	N	4025	SMA	O8-C8-C7	2.21	124.07	119.25
21	D	4014	7PH	O31-C31-O32	2.20	129.15	123.59
21	O	4114	7PH	O31-C31-O32	2.20	129.15	123.59
17	C	4005	SMA	O1-C2-C9	-2.20	109.30	111.91
21	D	4014	7PH	O31-C31-C32	-2.19	105.04	111.91
15	L	4121	UMQ	O1'-C1'-C2'	2.18	111.71	108.30
16	W	4026	HEM	CBA-CAA-C2A	-2.15	108.52	112.49
15	A	4021	UMQ	O1'-C1'-C2'	2.12	111.61	108.30
21	D	4014	7PH	O31-C3-C2	-2.10	102.32	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	4033	CN5	C36-C35-C34	2.05	124.85	114.42
17	N	4025	SMA	C7-C8-C8A	-2.05	118.38	120.18
20	C	4033	CN5	P-O11-C1	-2.03	111.58	121.59
17	C	4005	SMA	O8-C8-C7	2.02	123.66	119.25
15	A	4021	UMQ	C1-O5-C5	-2.01	109.74	113.69
22	D	4031	CN3	CC-CB-CA	-2.01	106.87	112.79
16	C	4001	HEM	CMB-C2B-C3B	2.00	128.43	124.68

There are no chirality outliers.

All (236) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	N	4111	9PE	C1-O11-P-O12
19	N	4111	9PE	C1-O11-P-O13
19	N	4111	9PE	C1-O11-P-O14
19	N	4111	9PE	O13-C11-C12-N
22	D	4031	CN3	C1-O11-P-O14
22	D	4031	CN3	CC-O13-P-O12
22	D	4031	CN3	CC-O13-P-O14
22	D	4031	CN3	O11-C1-C2-O21
22	D	4031	CN3	C22-C21-O21-C2
22	D	4031	CN3	O1'-C1'-C2'-O51
22	D	4031	CN3	C52-C51-O51-C2'
22	N	4131	CN3	C1-O11-P-O14
22	N	4131	CN3	CC-O13-P-O12
22	N	4131	CN3	CC-O13-P-O14
22	N	4131	CN3	O11-C1-C2-O21
22	N	4131	CN3	C22-C21-O21-C2
22	N	4131	CN3	O1'-C1'-C2'-O51
22	N	4131	CN3	C52-C51-O51-C2'
20	C	4033	CN5	CB-CC-O13-P
19	C	4011	9PE	C1-O11-P-O12
19	C	4011	9PE	C1-O11-P-O13
19	C	4011	9PE	C1-O11-P-O14
19	C	4011	9PE	C11-O13-P-O14
22	D	4031	CN3	O32-C31-O31-C3
22	D	4031	CN3	O22-C21-O21-C2
22	D	4031	CN3	O52-C51-O51-C2'
22	N	4131	CN3	O22-C21-O21-C2
22	N	4131	CN3	O52-C51-O51-C2'
22	D	4031	CN3	C32-C31-O31-C3
22	N	4131	CN3	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
20	C	4033	CN5	C32-C31-O31-C3
22	N	4131	CN3	O32-C31-O31-C3
20	C	4033	CN5	O3'-CA-CB-OA
15	A	4021	UMQ	O1'-CA-CB-CC
20	C	4033	CN5	O32-C31-O31-C3
15	L	4121	UMQ	O1'-CA-CB-CC
20	C	4033	CN5	O3'-CA-CB-CC
18	N	4110	8PE	C21-C22-C23-C24
22	D	4031	CN3	C43-C44-C45-C46
21	O	4114	7PH	C31-C32-C33-C34
21	D	4014	7PH	C21-C22-C23-C24
18	C	4010	8PE	C21-C22-C23-C24
21	D	4014	7PH	C31-C32-C33-C34
22	D	4031	CN3	O3'-CA-CB-OA
22	N	4131	CN3	O3'-CA-CB-OA
22	N	4131	CN3	C41-C42-C43-C44
14	L	4113	6PH	C22-C21-O21-C2
22	D	4031	CN3	CC-O13-P-O11
22	D	4031	CN3	CA-O3'-P'-O1'
22	N	4131	CN3	CC-O13-P-O11
22	N	4131	CN3	CA-O3'-P'-O1'
19	C	4011	9PE	C11-O13-P-O11
22	D	4031	CN3	O3'-CA-CB-CC
22	N	4131	CN3	O3'-CA-CB-CC
14	L	4113	6PH	O22-C21-O21-C2
20	C	4033	CN5	C3A-C3B-C3C-C3D
22	D	4031	CN3	C52-C53-C54-C55
14	L	4113	6PH	C37-C38-C39-C3A
18	N	4110	8PE	C32-C33-C34-C35
18	N	4110	8PE	C36-C37-C38-C39
18	C	4010	8PE	C37-C38-C39-C3A
19	C	4011	9PE	C2E-C2F-C2G-C2H
21	D	4014	7PH	C32-C33-C34-C35
14	A	4013	6PH	C27-C28-C29-C2A
18	N	4110	8PE	C3A-C3B-C3C-C3D
21	O	4114	7PH	C27-C28-C29-C2A
22	N	4131	CN3	C55-C56-C57-C58
21	D	4014	7PH	C37-C38-C39-C3A
20	C	4033	CN5	C37-C38-C39-C3A
19	N	4111	9PE	C2C-C2D-C2E-C2F
21	D	4014	7PH	C22-C23-C24-C25
22	D	4031	CN3	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
18	N	4110	8PE	C2A-C2B-C2C-C2D
21	O	4114	7PH	C32-C33-C34-C35
22	N	4131	CN3	C46-C47-C48-C49
19	N	4111	9PE	C2E-C2F-C2G-C2H
14	A	4013	6PH	C39-C3A-C3B-C3C
18	N	4110	8PE	C35-C36-C37-C38
21	D	4014	7PH	C2A-C2B-C2C-C2D
22	D	4031	CN3	C42-C43-C44-C45
15	A	4021	UMQ	CF-CG-CH-CI
14	L	4113	6PH	C36-C37-C38-C39
18	N	4110	8PE	C33-C34-C35-C36
15	L	4121	UMQ	CD-CF-CG-CH
21	O	4114	7PH	C37-C38-C39-C3A
19	C	4011	9PE	C26-C27-C28-C29
18	N	4110	8PE	O11-C1-C2-C3
18	C	4010	8PE	O11-C1-C2-C3
20	C	4033	CN5	C3B-C3C-C3D-C3E
14	L	4113	6PH	C32-C33-C34-C35
19	C	4011	9PE	C22-C23-C24-C25
21	D	4014	7PH	C27-C28-C29-C2A
20	C	4033	CN5	C39-C3A-C3B-C3C
19	C	4011	9PE	C2D-C2E-C2F-C2G
19	N	4111	9PE	C28-C29-C2A-C2B
14	L	4113	6PH	C35-C36-C37-C38
18	N	4110	8PE	C3C-C3D-C3E-C3F
19	C	4011	9PE	C28-C29-C2A-C2B
14	A	4013	6PH	C34-C35-C36-C37
21	O	4114	7PH	C22-C23-C24-C25
18	C	4010	8PE	C29-C2A-C2B-C2C
20	C	4033	CN5	C42-C41-O41-C3'
14	A	4013	6PH	O22-C21-O21-C2
19	N	4111	9PE	C26-C27-C28-C29
14	A	4013	6PH	C35-C36-C37-C38
21	O	4114	7PH	C26-C27-C28-C29
18	N	4110	8PE	C31-C32-C33-C34
14	L	4113	6PH	C38-C39-C3A-C3B
19	N	4111	9PE	C22-C23-C24-C25
14	A	4013	6PH	C22-C21-O21-C2
14	A	4013	6PH	C29-C2A-C2B-C2C
14	A	4013	6PH	C2B-C2C-C2D-C2E
18	N	4110	8PE	C26-C27-C28-C29
14	A	4013	6PH	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
14	A	4013	6PH	C25-C26-C27-C28
18	N	4110	8PE	C3B-C3C-C3D-C3E
18	N	4110	8PE	C23-C24-C25-C26
18	C	4010	8PE	C3B-C3C-C3D-C3E
17	C	4005	SMA	C4A-C5-O5-C5M
18	C	4010	8PE	C32-C33-C34-C35
19	N	4111	9PE	O11-C1-C2-C3
22	D	4031	CN3	O11-C1-C2-C3
22	D	4031	CN3	O1'-C1'-C2'-C3'
22	N	4131	CN3	O11-C1-C2-C3
22	N	4131	CN3	O1'-C1'-C2'-C3'
19	C	4011	9PE	O11-C1-C2-C3
22	N	4131	CN3	C47-C48-C49-C4A
18	N	4110	8PE	C38-C39-C3A-C3B
14	L	4113	6PH	C28-C29-C2A-C2B
19	N	4111	9PE	C29-C2A-C2B-C2C
19	N	4111	9PE	C21-C22-C23-C24
17	C	4005	SMA	C9-C10-C11-C22
14	L	4113	6PH	C29-C2A-C2B-C2C
15	L	4121	UMQ	CF-CG-CH-CI
19	N	4111	9PE	C2A-C2B-C2C-C2D
21	D	4014	7PH	C26-C27-C28-C29
14	L	4113	6PH	C27-C28-C29-C2A
17	C	4005	SMA	C6-C5-O5-C5M
21	D	4014	7PH	C2B-C2C-C2D-C2E
15	A	4021	UMQ	CI-CJ-CK-CL
21	O	4114	7PH	C2A-C2B-C2C-C2D
14	A	4013	6PH	C32-C33-C34-C35
20	C	4033	CN5	O11-C1-C2-C3
20	C	4033	CN5	O1'-C1'-C2'-C3'
20	C	4033	CN5	C38-C39-C3A-C3B
18	C	4010	8PE	C35-C36-C37-C38
15	A	4021	UMQ	CD-CF-CG-CH
14	A	4013	6PH	C36-C37-C38-C39
22	N	4131	CN3	C56-C57-C58-C59
20	C	4033	CN5	C35-C36-C37-C38
18	C	4010	8PE	C34-C35-C36-C37
18	C	4010	8PE	C33-C34-C35-C36
22	D	4031	CN3	C47-C48-C49-C4A
19	C	4011	9PE	C24-C25-C26-C27
22	D	4031	CN3	C1-O11-P-O13
14	L	4113	6PH	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
19	N	4111	9PE	O11-C1-C2-O21
19	C	4011	9PE	O11-C1-C2-O21
22	D	4031	CN3	C21-C22-C23-C24
22	N	4131	CN3	C21-C22-C23-C24
15	L	4121	UMQ	CG-CH-CI-CJ
18	C	4010	8PE	C28-C29-C2A-C2B
19	C	4011	9PE	O31-C31-C32-C33
22	D	4031	CN3	C45-C46-C47-C48
20	C	4033	CN5	CB-CA-O3'-P'
19	N	4111	9PE	C24-C25-C26-C27
21	D	4014	7PH	C36-C37-C38-C39
20	C	4033	CN5	O42-C41-O41-C3'
18	N	4110	8PE	C29-C2A-C2B-C2C
18	C	4010	8PE	C2A-C2B-C2C-C2D
18	C	4010	8PE	C36-C37-C38-C39
21	O	4114	7PH	C22-C21-O21-C2
14	L	4113	6PH	O11-C1-C2-O21
18	N	4110	8PE	O11-C1-C2-O21
18	C	4010	8PE	O11-C1-C2-O21
21	O	4114	7PH	O22-C21-O21-C2
18	C	4010	8PE	C3A-C3B-C3C-C3D
22	N	4131	CN3	C44-C45-C46-C47
18	N	4110	8PE	C3D-C3E-C3F-C3G
22	D	4031	CN3	CA-O3'-P'-O2'
22	N	4131	CN3	CA-O3'-P'-O2'
19	C	4011	9PE	C11-O13-P-O12
14	A	4013	6PH	O11-C1-C2-C3
14	L	4113	6PH	O11-C1-C2-C3
14	L	4113	6PH	C2C-C2D-C2E-C2F
19	N	4111	9PE	O31-C31-C32-C33
19	C	4011	9PE	C23-C24-C25-C26
22	D	4031	CN3	C46-C47-C48-C49
22	N	4131	CN3	C53-C54-C55-C56
14	L	4113	6PH	C25-C26-C27-C28
20	C	4033	CN5	C31-C32-C33-C34
22	D	4031	CN3	C1'-O1'-P'-O3'
22	N	4131	CN3	C1-O11-P-O13
22	N	4131	CN3	C1'-O1'-P'-O3'
18	N	4110	8PE	C11-O13-P-O11
18	C	4010	8PE	C11-O13-P-O11
19	N	4111	9PE	C23-C24-C25-C26
18	C	4010	8PE	C3C-C3D-C3E-C3F

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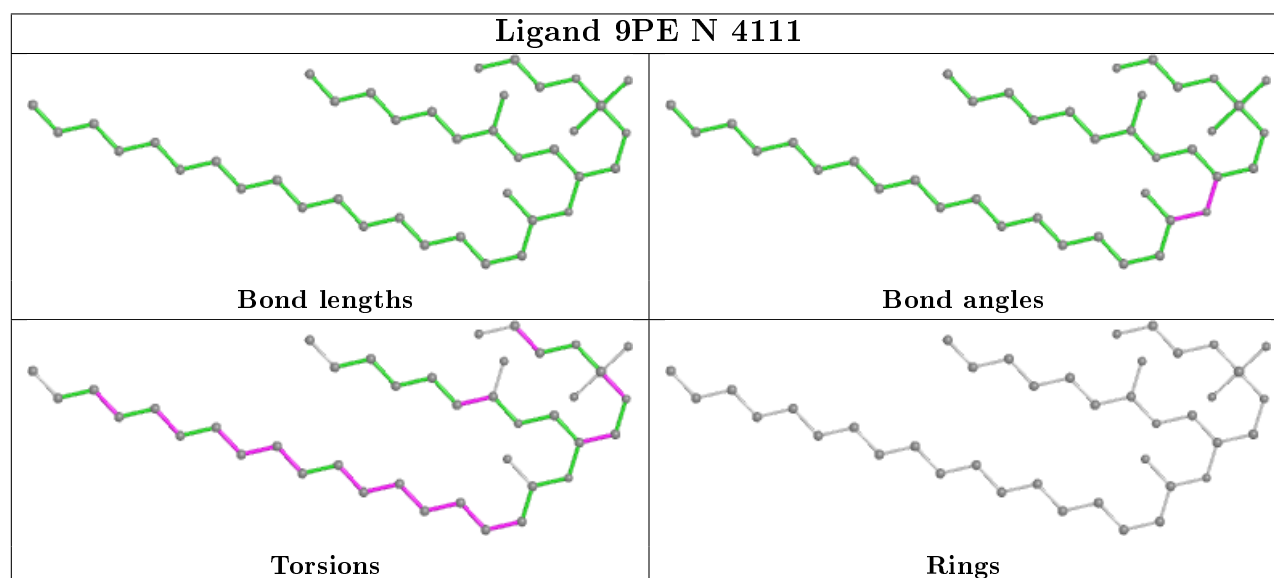
Mol	Chain	Res	Type	Atoms
21	D	4014	7PH	C23-C24-C25-C26
18	C	4010	8PE	C3E-C3F-C3G-C3H
14	A	4013	6PH	C28-C29-C2A-C2B
22	N	4131	CN3	C43-C44-C45-C46
22	D	4031	CN3	C41-C42-C43-C44
19	C	4011	9PE	C27-C28-C29-C2A
21	O	4114	7PH	C34-C35-C36-C37
14	A	4013	6PH	C24-C25-C26-C27
19	C	4011	9PE	C2B-C2C-C2D-C2E
14	L	4113	6PH	C3A-C3B-C3C-C3D
21	O	4114	7PH	C38-C39-C3A-C3B
21	O	4114	7PH	C21-C22-C23-C24
19	C	4011	9PE	C21-C22-C23-C24
18	N	4110	8PE	C28-C29-C2A-C2B
14	L	4113	6PH	C33-C34-C35-C36
14	A	4013	6PH	O31-C31-C32-C33
20	C	4033	CN5	C1-O11-P-O13
14	L	4113	6PH	O31-C31-C32-C33
18	N	4110	8PE	C27-C28-C29-C2A
22	N	4131	CN3	C48-C49-C4A-C4B
18	N	4110	8PE	C37-C38-C39-C3A
22	D	4031	CN3	O31-C31-C32-C33
21	D	4014	7PH	C33-C34-C35-C36
22	D	4031	CN3	C54-C55-C56-C57
19	C	4011	9PE	O32-C31-C32-C33
14	A	4013	6PH	O32-C31-C32-C33
14	L	4113	6PH	O32-C31-C32-C33
22	D	4031	CN3	CA-O3'-P'-O4'
20	C	4033	CN5	C1-O11-P-O14
22	N	4131	CN3	C51-C52-C53-C54
18	C	4010	8PE	C12-C11-O13-P
19	C	4011	9PE	C2C-C2D-C2E-C2F
21	D	4014	7PH	C29-C2A-C2B-C2C
18	C	4010	8PE	C27-C28-C29-C2A
19	N	4111	9PE	C25-C26-C27-C28
22	N	4131	CN3	O51-C51-C52-C53
14	A	4013	6PH	C37-C38-C39-C3A
18	N	4110	8PE	O31-C31-C32-C33

There are no ring outliers.

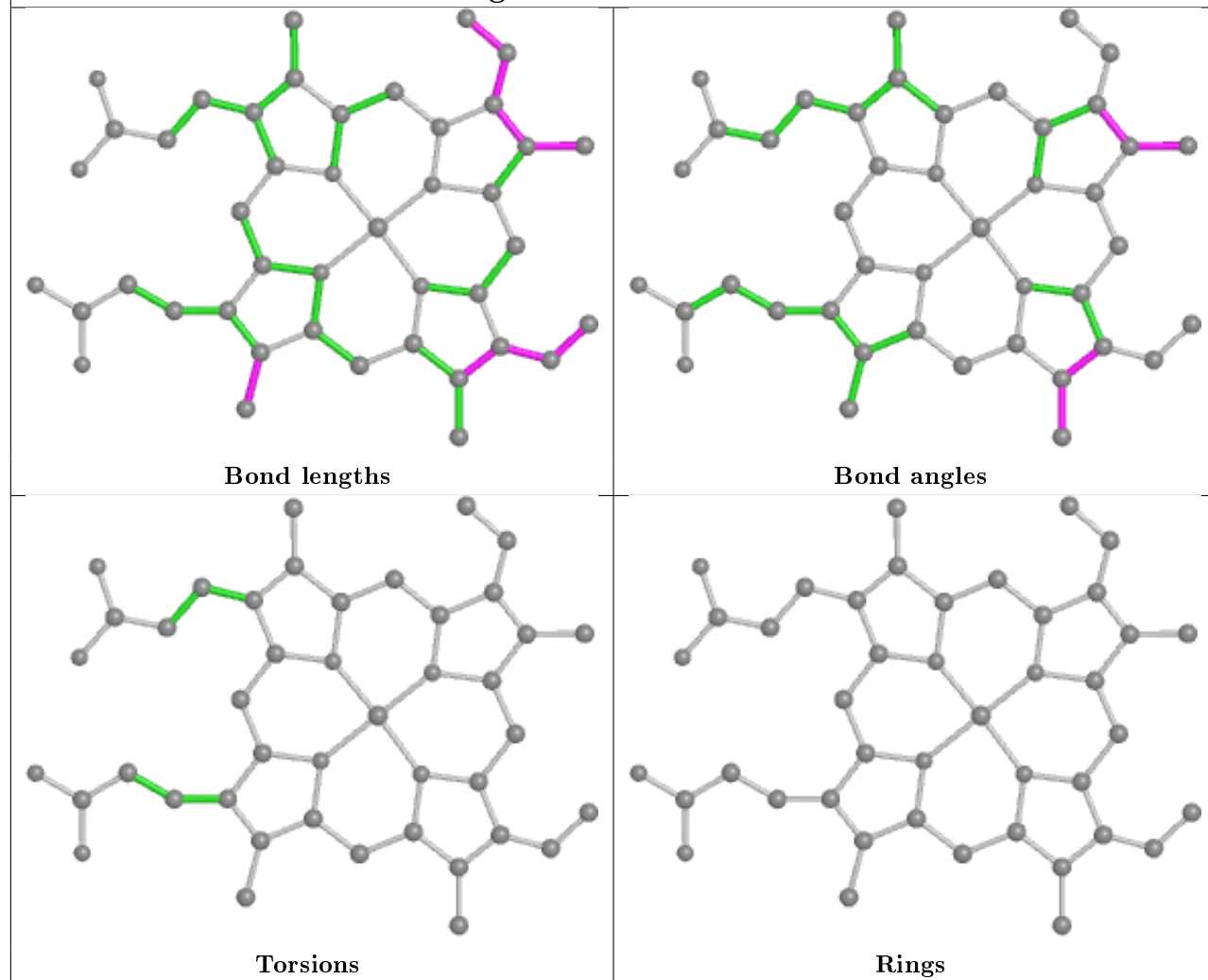
16 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	N	4022	HEM	1	0
21	D	4014	7PH	2	0
22	D	4031	CN3	5	0
14	A	4013	6PH	1	0
22	N	4131	CN3	5	0
15	A	4021	UMQ	2	0
20	C	4033	CN5	5	0
14	L	4113	6PH	3	0
16	C	4001	HEM	1	0
16	C	4002	HEM	1	0
17	C	4005	SMA	1	0
15	L	4121	UMQ	2	0
18	C	4010	8PE	1	0
21	O	4114	7PH	2	0
16	N	4021	HEM	2	0
16	D	4003	HEM	1	0

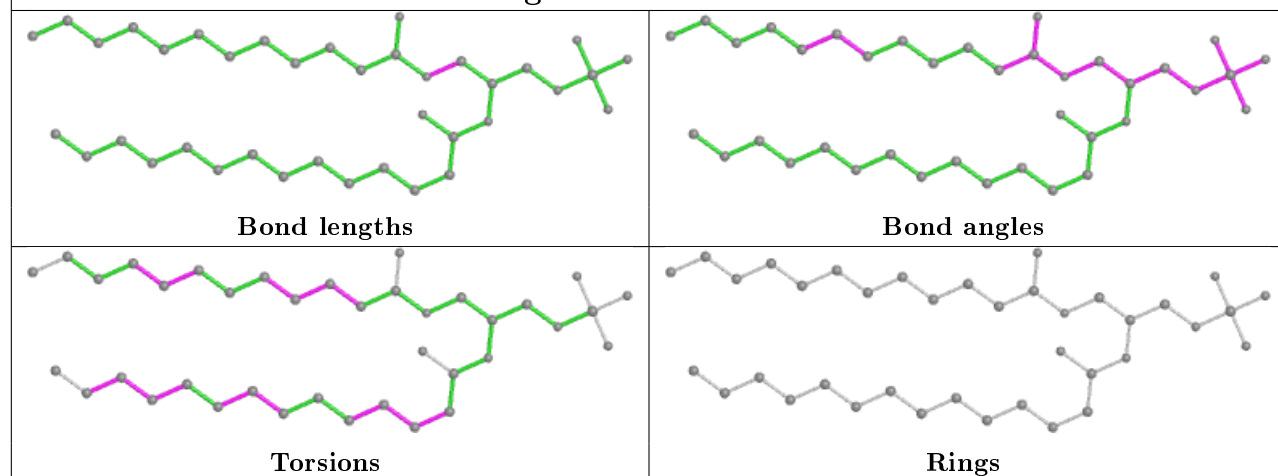
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

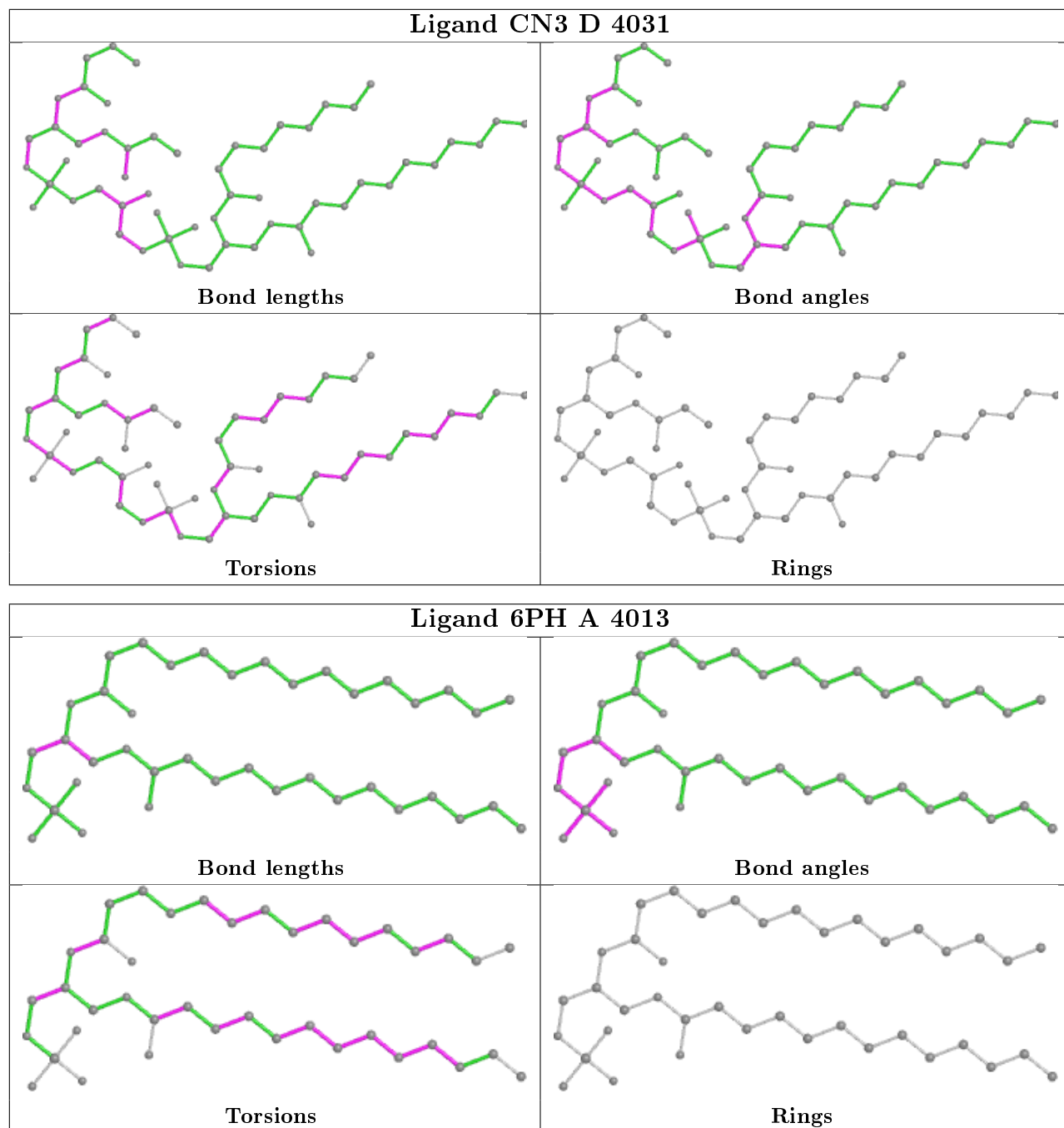


## Ligand HEM N 4022

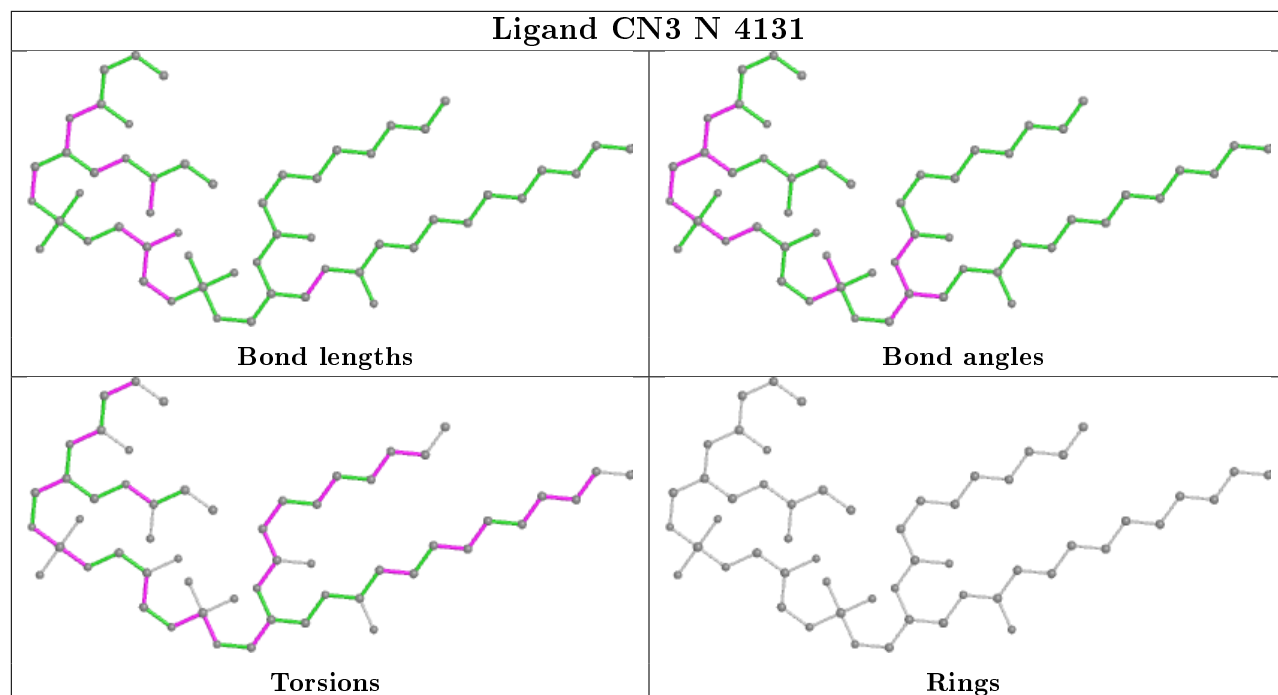


## Ligand 7PH D 4014

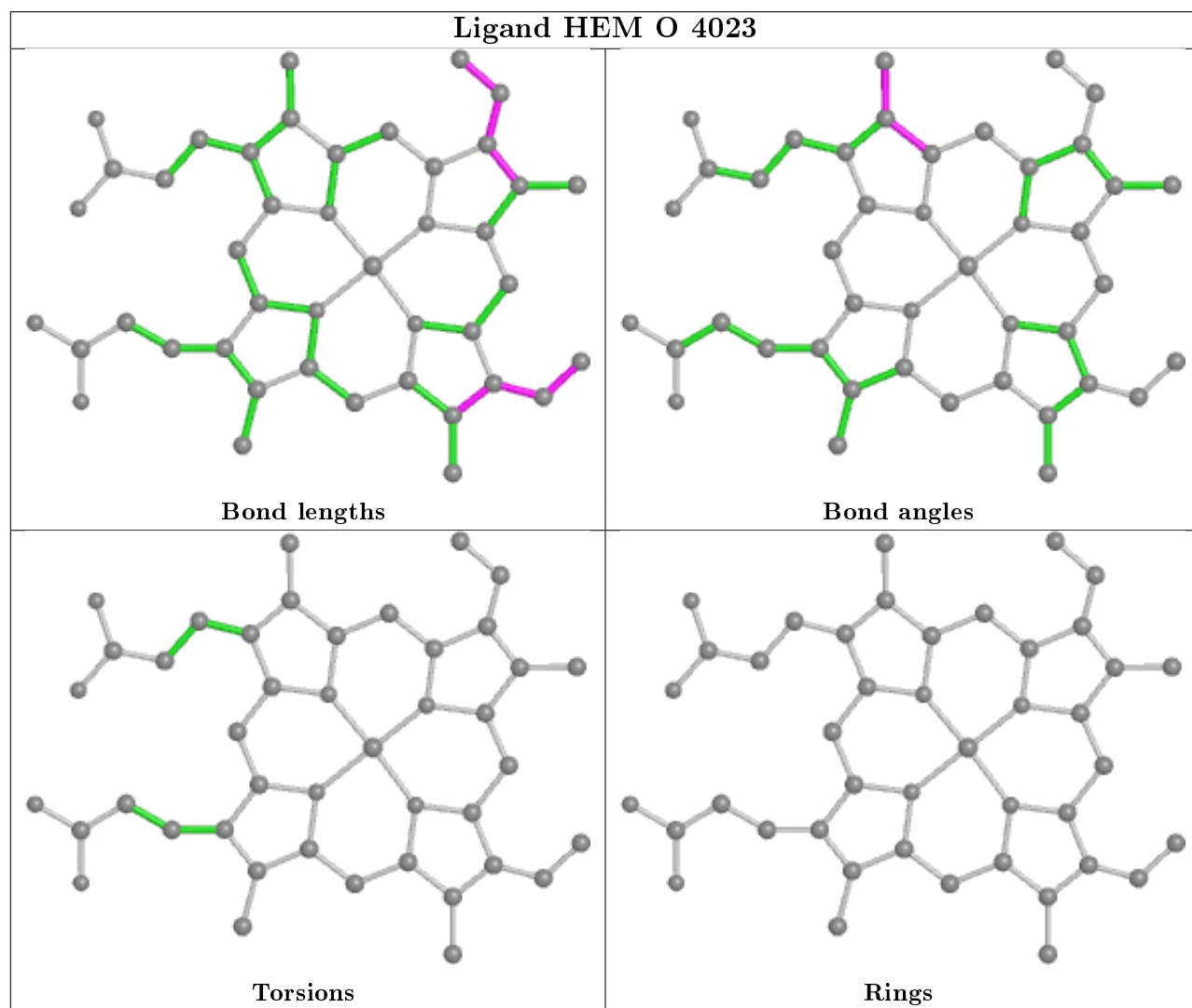


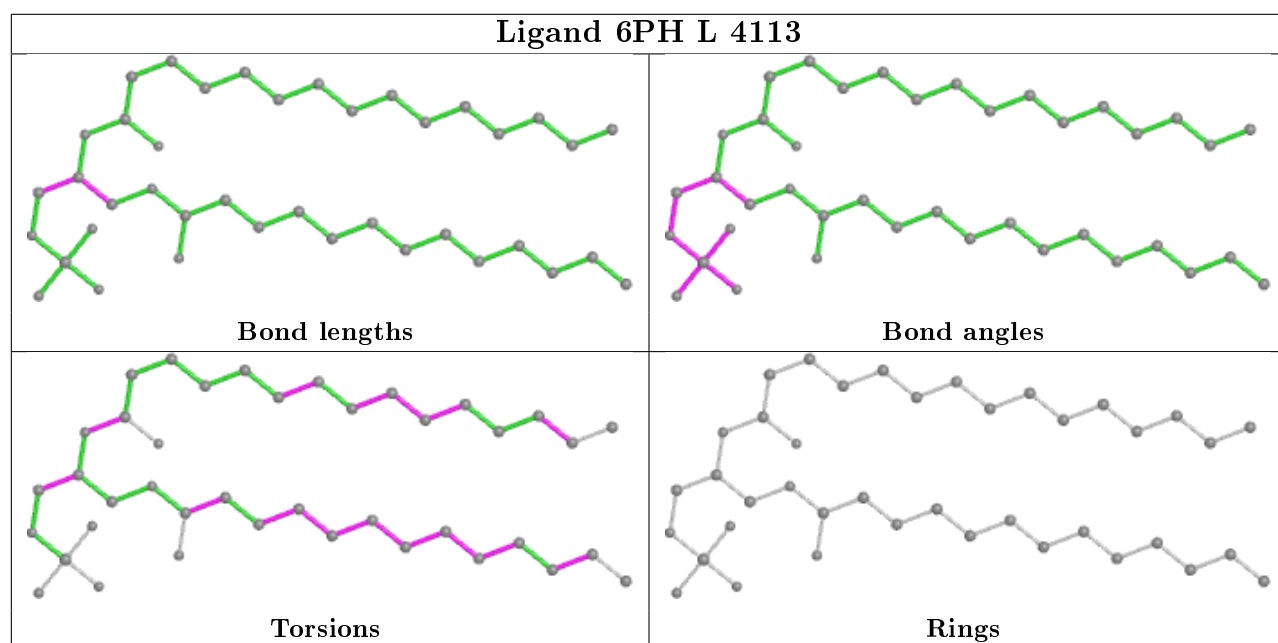
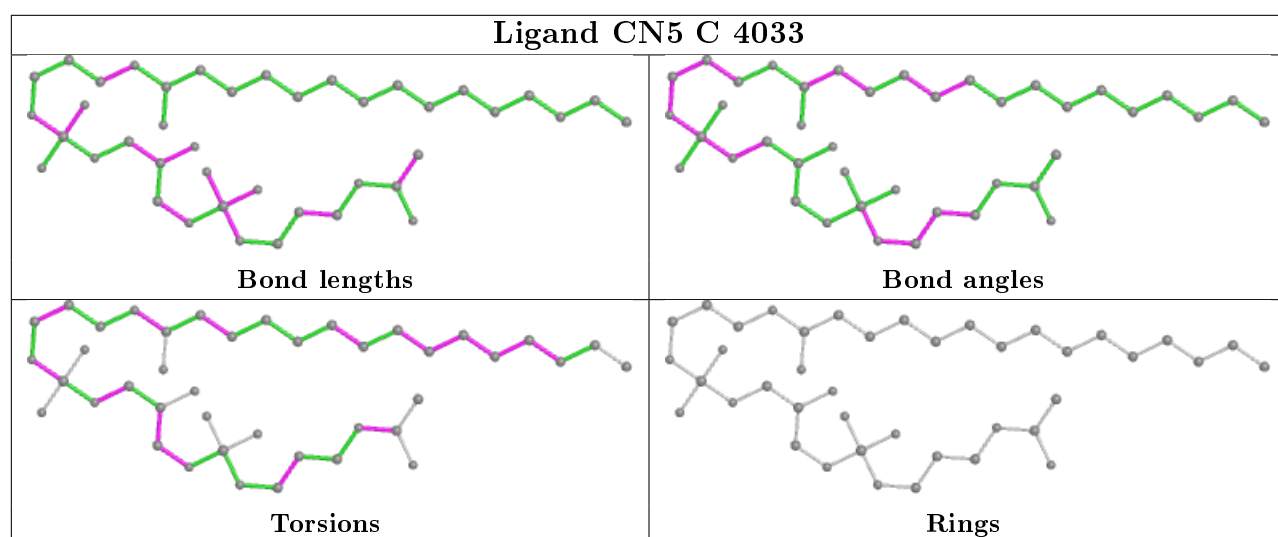
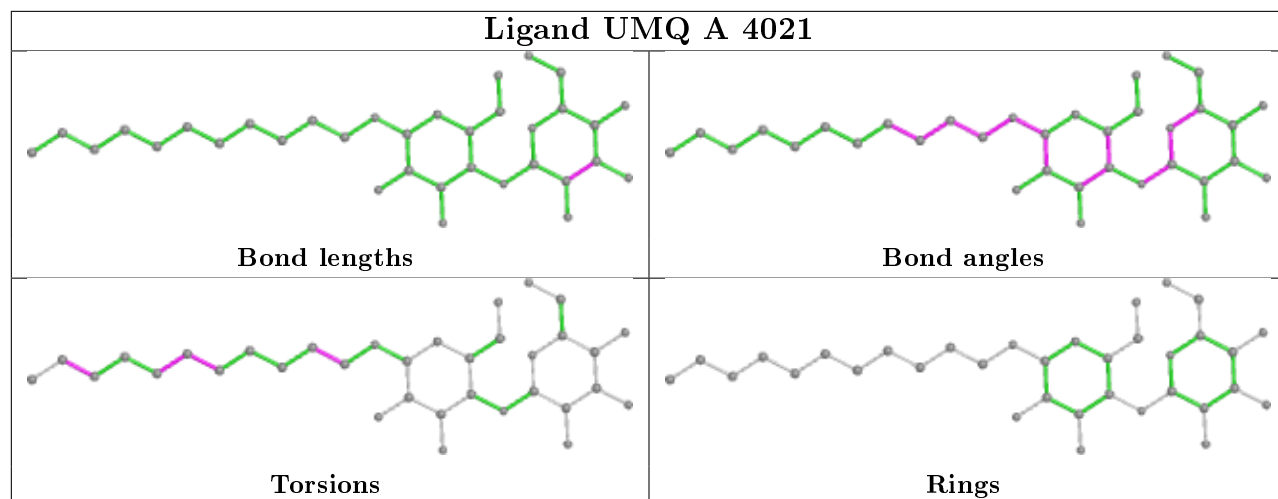


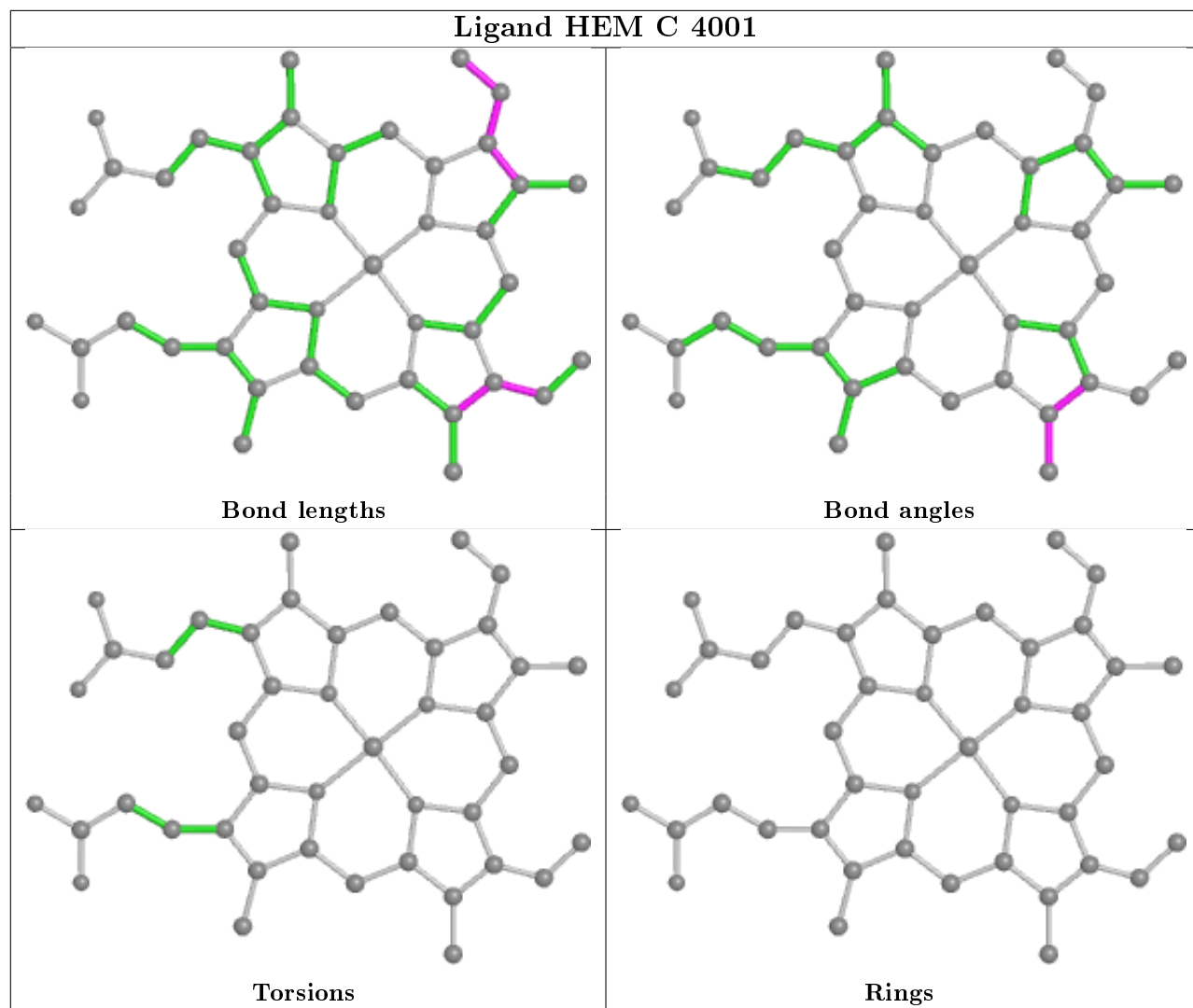
## Ligand CN3 N 4131



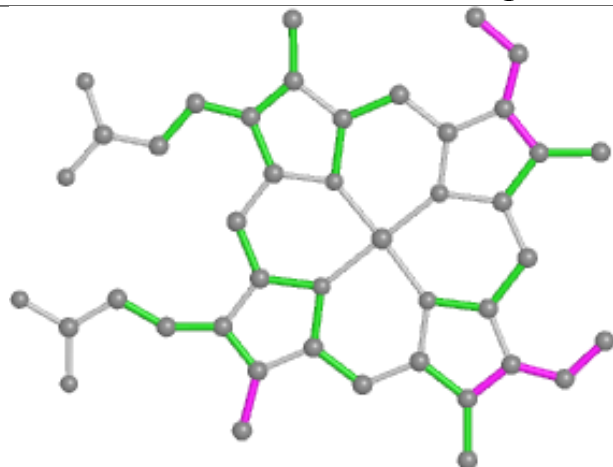
## Ligand HEM O 4023



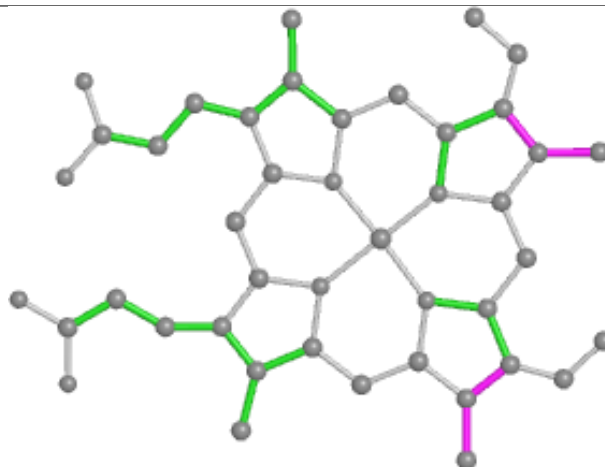




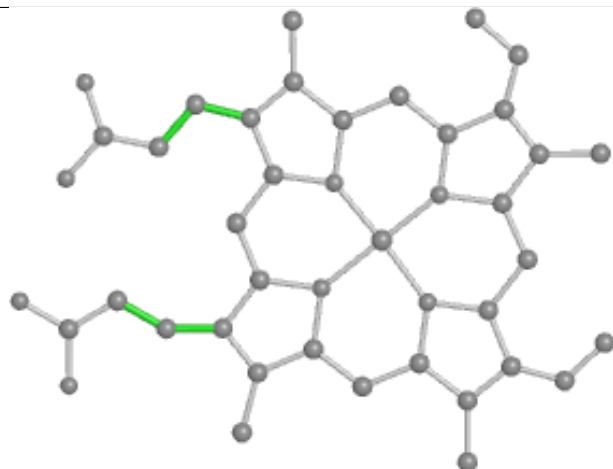
## Ligand HEM C 4002



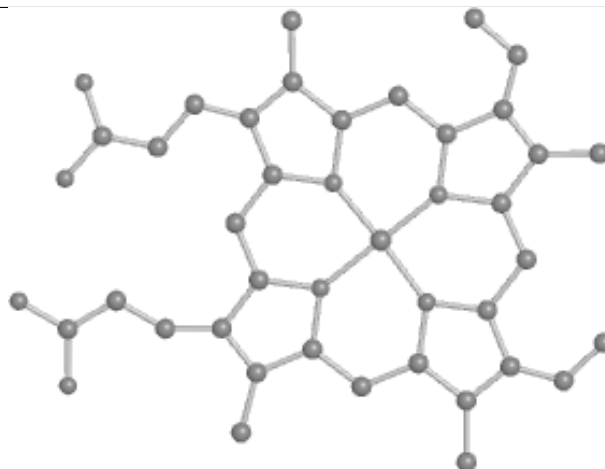
Bond lengths



Bond angles

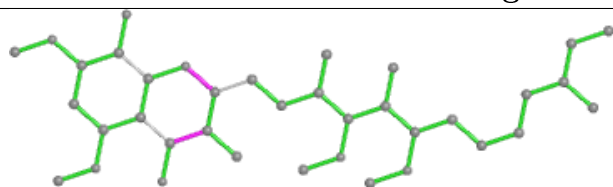


Torsions

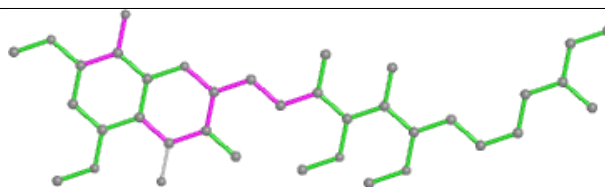


Rings

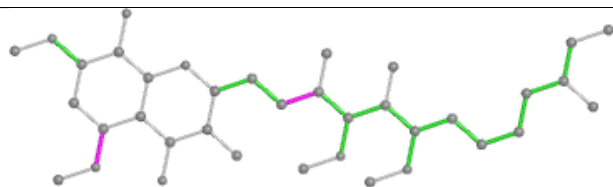
## Ligand SMA C 4005



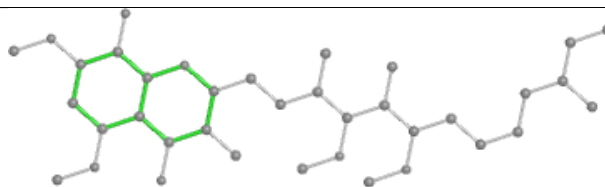
Bond lengths



Bond angles

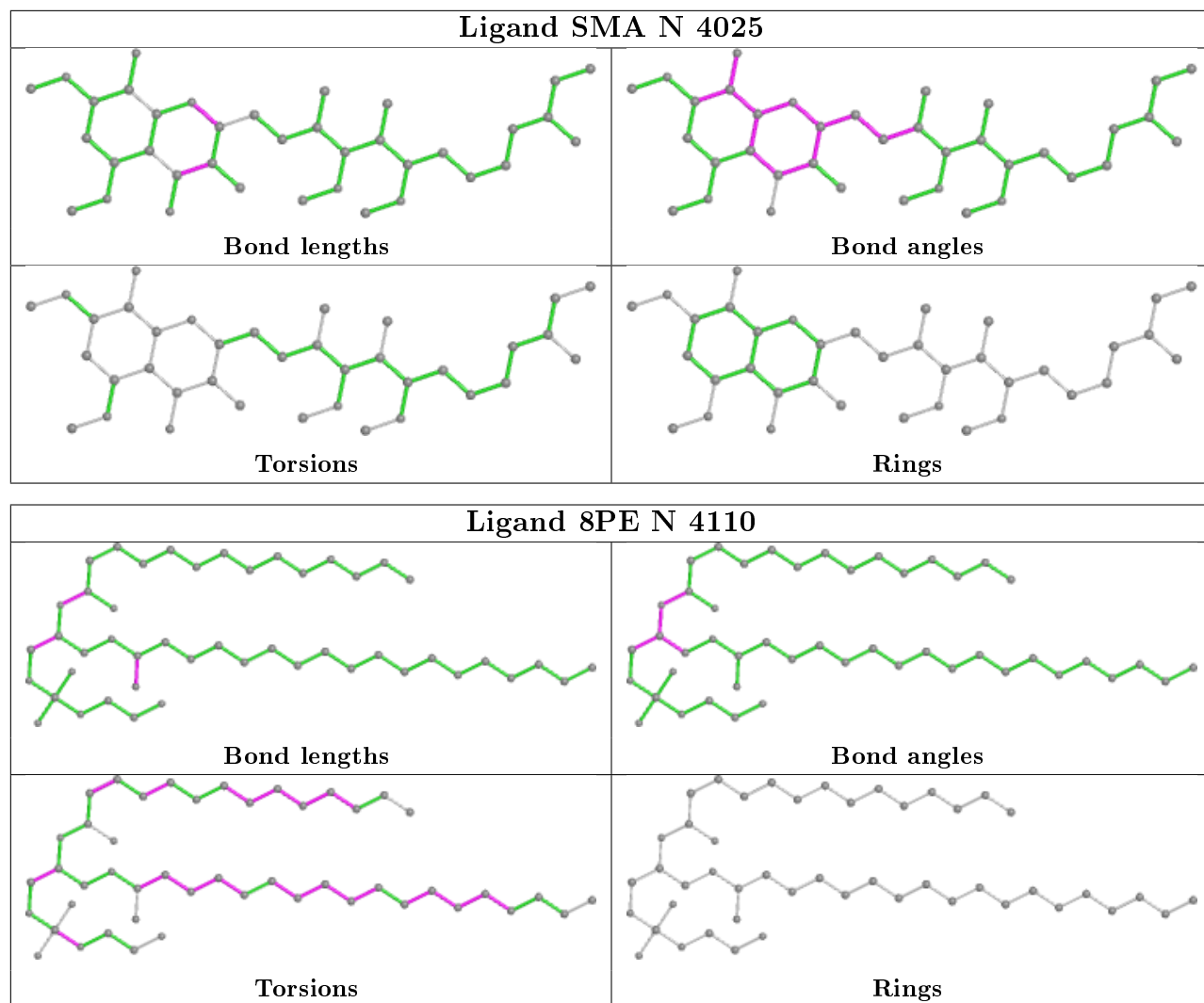


Torsions

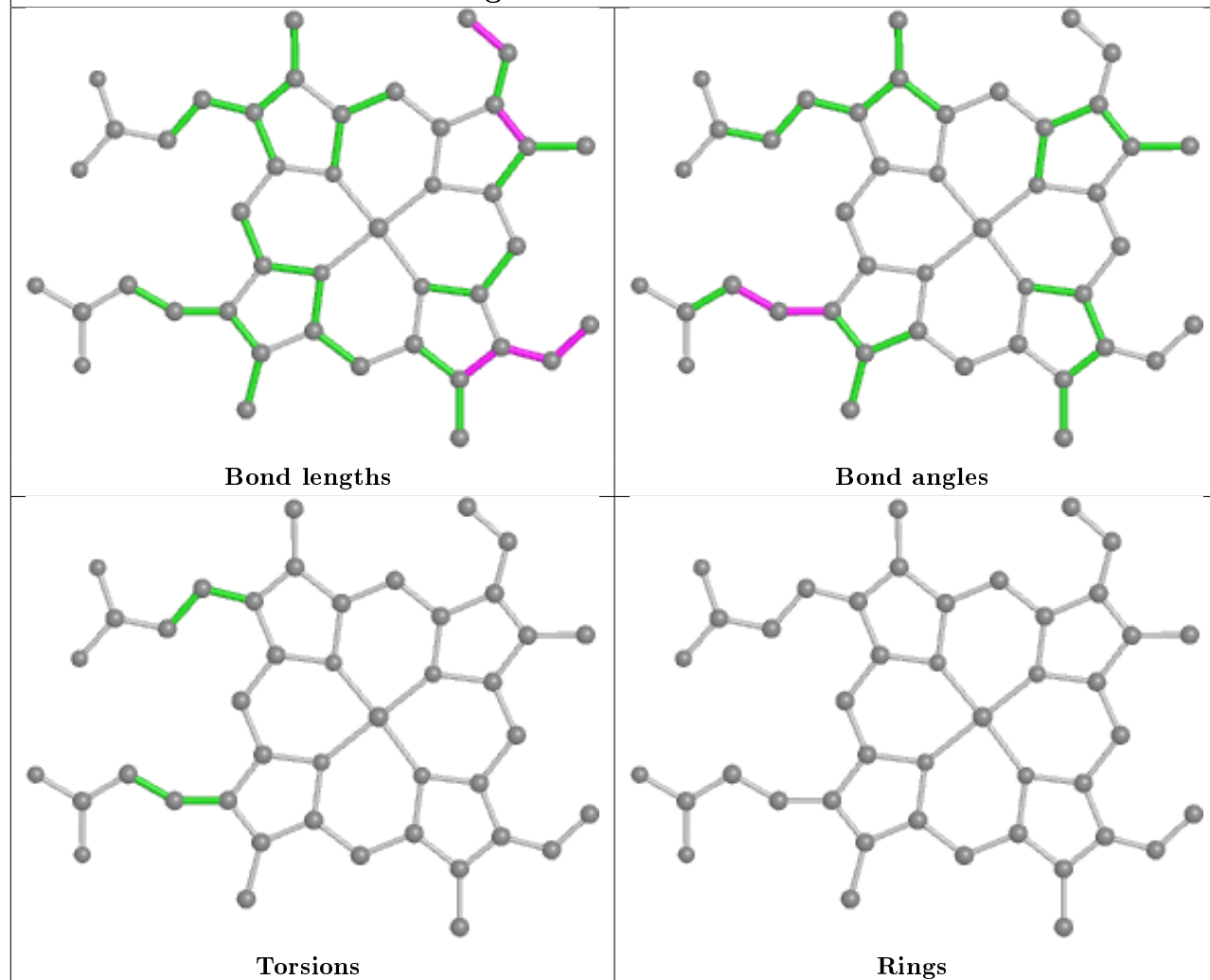


Rings

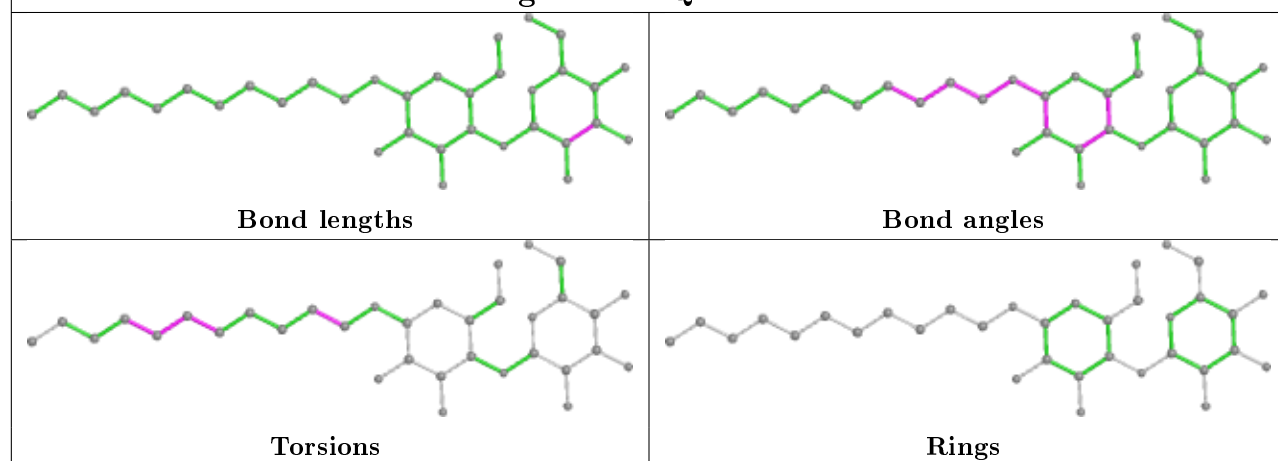


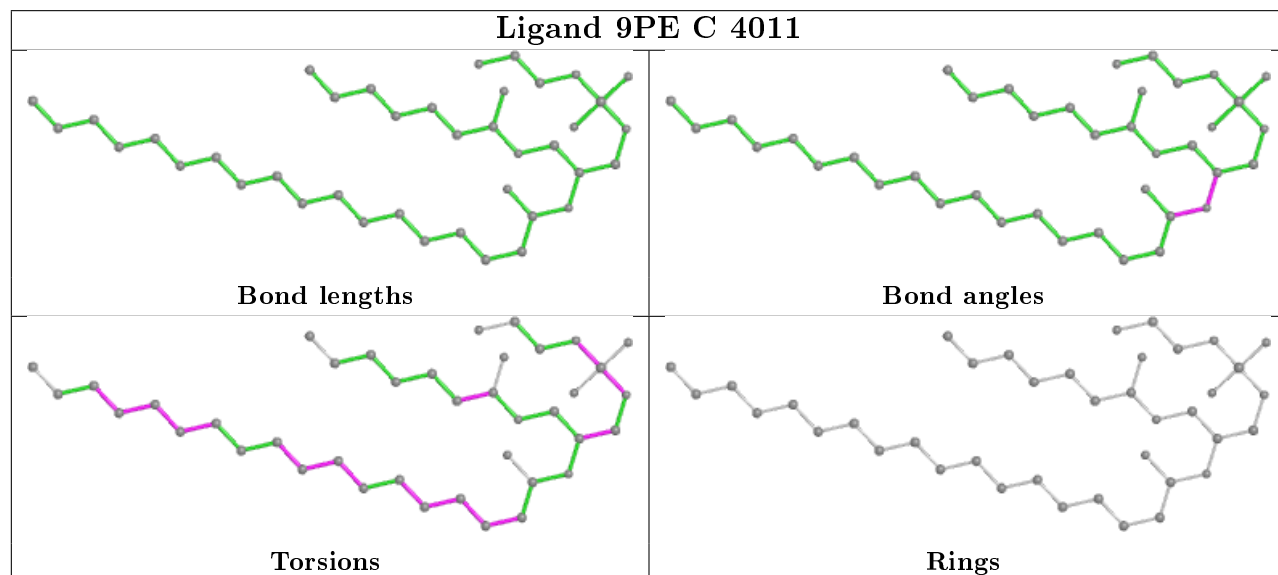
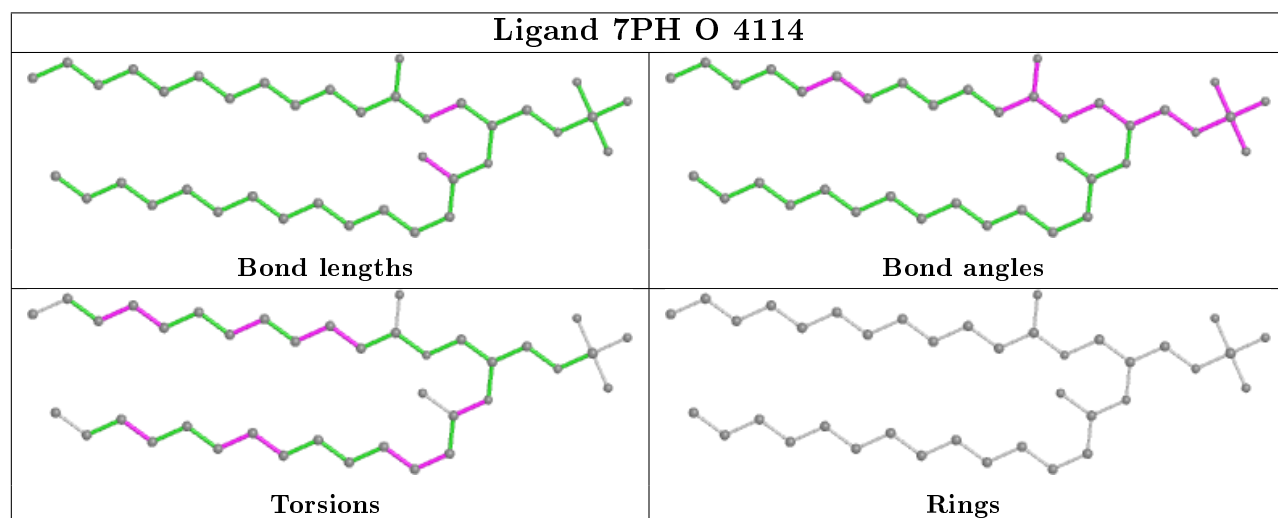
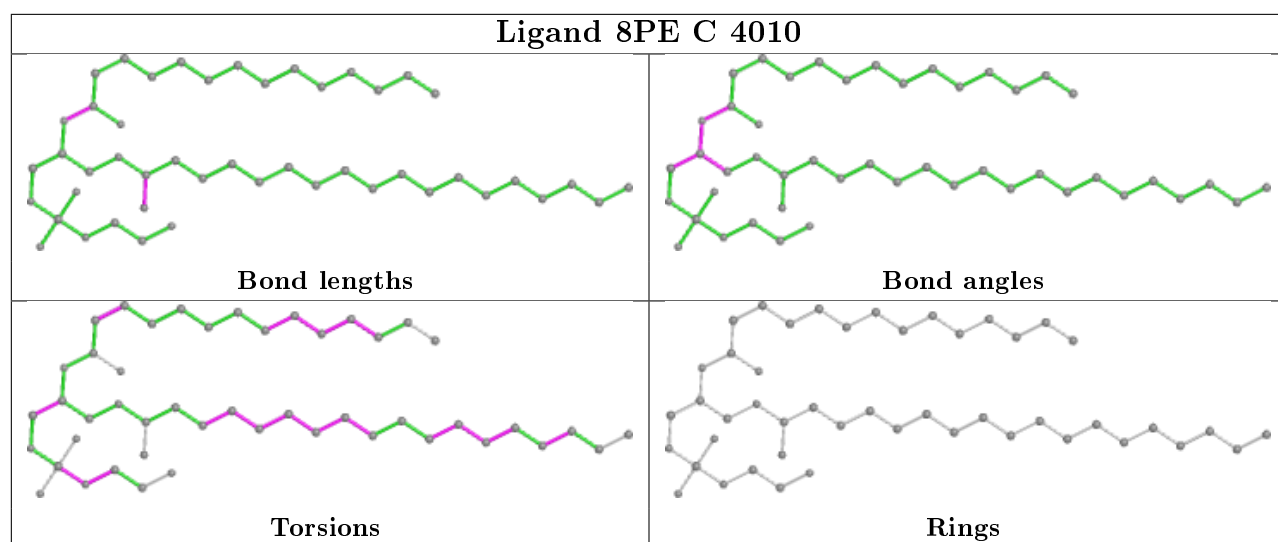


## Ligand HEM W 4026

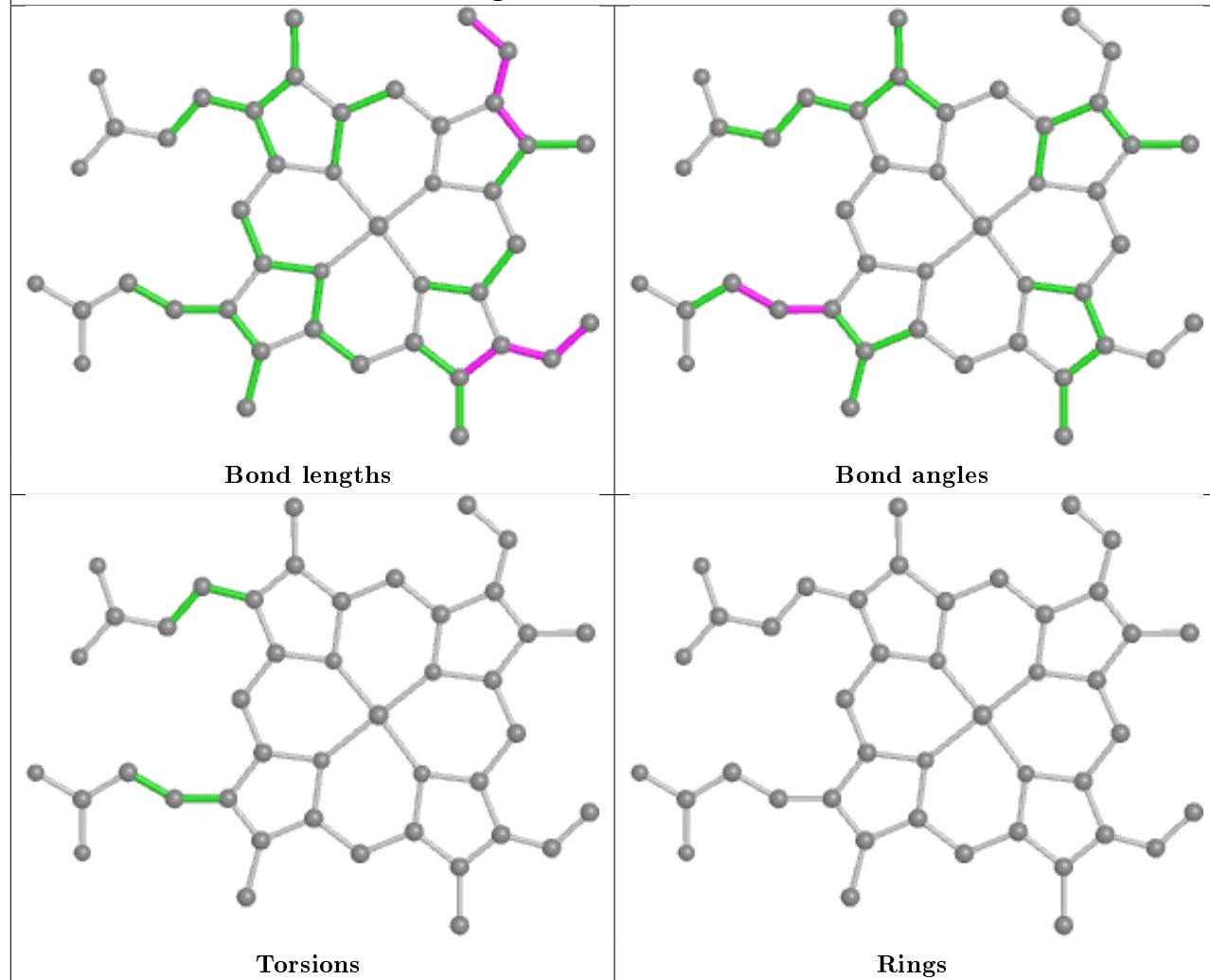


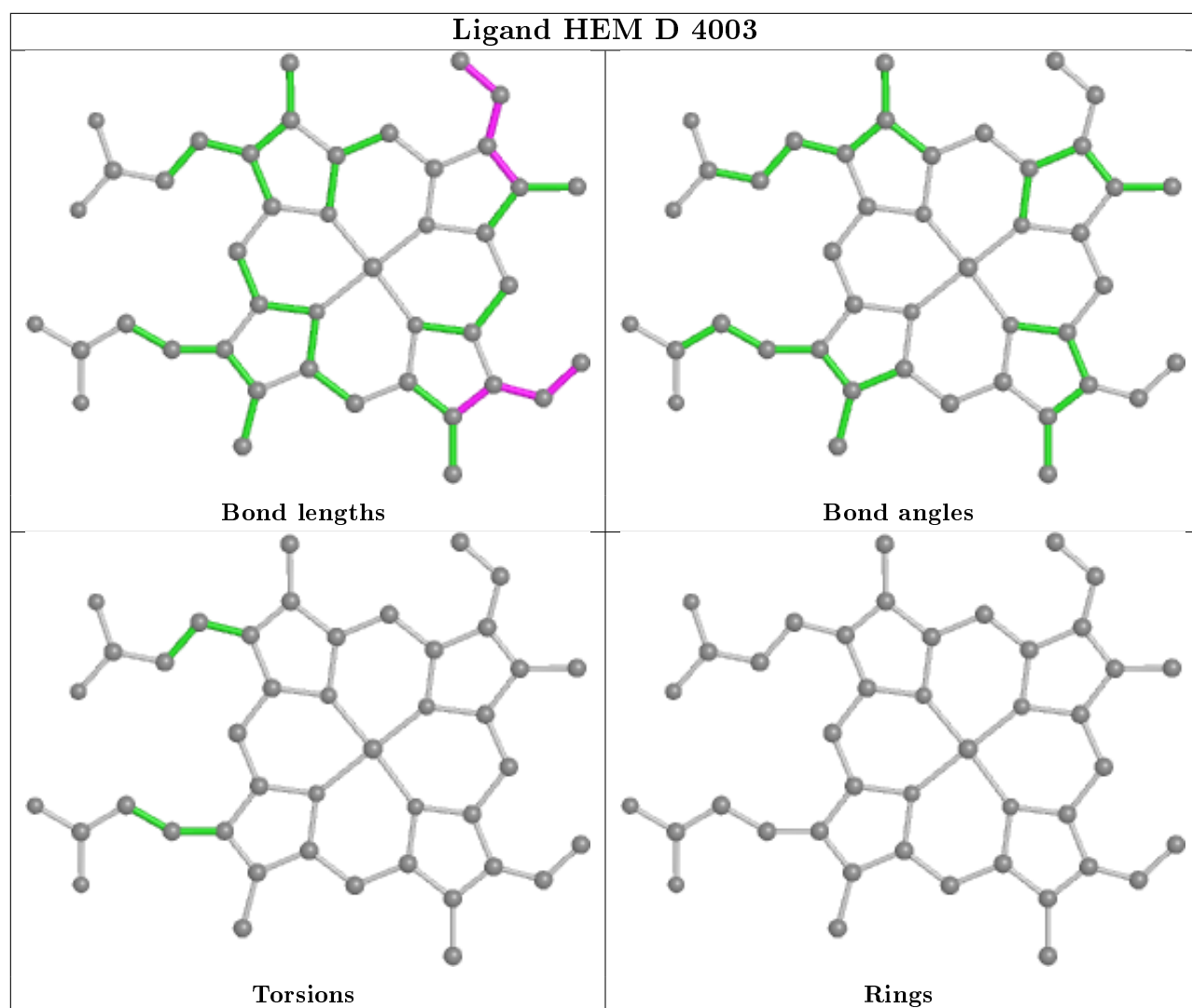
## Ligand UMQ L 4121





## Ligand HEM N 4021





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	431/431 (100%)	0.54	50 (11%) 4 5	26, 44, 98, 114	0
1	L	431/431 (100%)	0.46	40 (9%) 8 10	25, 42, 90, 113	0
2	B	352/352 (100%)	0.59	29 (8%) 11 13	30, 47, 73, 114	0
2	M	352/352 (100%)	0.54	36 (10%) 6 8	32, 45, 72, 109	0
3	C	385/385 (100%)	-0.17	4 (1%) 82 84	18, 27, 38, 91	0
3	N	385/385 (100%)	-0.22	4 (1%) 82 84	19, 26, 37, 88	0
4	D	248/248 (100%)	0.01	11 (4%) 34 37	25, 35, 57, 83	0
4	O	248/248 (100%)	-0.05	7 (2%) 53 56	24, 33, 55, 86	0
5	E	185/185 (100%)	0.45	14 (7%) 13 15	24, 40, 69, 94	0
5	P	185/185 (100%)	0.65	23 (12%) 4 4	24, 41, 80, 93	0
6	F	74/146 (50%)	0.82	12 (16%) 1 1	34, 46, 90, 96	0
6	Q	74/146 (50%)	0.78	13 (17%) 1 1	32, 45, 87, 90	0
7	G	126/126 (100%)	-0.04	7 (5%) 24 27	26, 37, 60, 78	0
7	R	126/126 (100%)	-0.02	6 (4%) 30 33	23, 34, 62, 80	0
8	H	93/93 (100%)	1.85	27 (29%) 0 0	24, 45, 128, 131	0
8	S	93/93 (100%)	1.29	21 (22%) 0 0	22, 43, 113, 119	0
9	I	57/65 (87%)	0.83	7 (12%) 4 4	34, 42, 83, 100	0
9	T	57/65 (87%)	0.76	7 (12%) 4 4	32, 40, 84, 96	0
10	J	127/127 (100%)	0.93	20 (15%) 2 2	40, 57, 71, 80	0
10	U	127/127 (100%)	1.12	22 (17%) 1 1	42, 59, 73, 82	0
11	K	107/107 (100%)	2.27	50 (46%) 0 0	51, 81, 114, 116	0
11	V	107/107 (100%)	2.82	67 (62%) 0 0	60, 92, 120, 122	0
12	W	107/108 (99%)	1.43	27 (25%) 0 0	46, 62, 87, 99	0
All	All	4477/4638 (96%)	0.52	504 (11%) 5 5	18, 41, 90, 131	0

All (504) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	46	PHE	19.6
2	B	338	LEU	18.4
1	L	230	LEU	17.9
9	I	57	ALA	13.6
9	T	58	ALA	13.5
1	A	27	ALA	12.5
8	H	42	HIS	12.1
1	A	228	LEU	11.1
8	H	49	PHE	11.0
8	H	45	VAL	10.9
9	I	58	ALA	10.9
8	S	49	PHE	10.6
12	W	1	THR	10.4
1	A	230	LEU	10.1
2	B	332	VAL	9.9
11	V	15	LEU	9.7
8	S	46	PHE	9.5
2	B	336	ILE	9.5
8	H	41	PHE	9.5
11	V	106	ILE	9.2
1	A	129	ALA	9.2
3	C	384	ASN	9.2
8	S	40	ILE	9.1
8	H	44	ALA	9.1
9	T	57	ALA	9.0
3	N	384	ASN	9.0
1	L	27	ALA	8.7
11	V	79	GLU	8.5
2	M	338	LEU	8.3
11	K	106	ILE	8.2
11	V	29	ILE	8.1
8	S	94	VAL	8.0
2	M	336	ILE	8.0
8	H	39	GLY	7.9
6	Q	119	HIS	7.8
1	A	128	LYS	7.7
8	S	41	PHE	7.5
1	L	227	ASN	7.5
8	H	94	VAL	7.5
8	H	40	ILE	7.4
8	H	52	PHE	7.4
3	C	383	VAL	7.4

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Mol	Chain	Res	Type	RSRZ
6	F	119	HIS	7.4
5	E	47	ASN	7.3
8	H	43	ASN	7.3
11	V	14	SER	7.2
8	H	51	ARG	7.2
8	S	38	GLN	7.2
1	L	229	SER	7.2
2	M	330	GLU	7.1
11	K	11	LEU	7.1
8	H	37	LEU	7.0
1	A	234	THR	7.0
11	K	9	VAL	7.0
9	I	2	SER	7.0
8	H	47	ASN	7.0
4	O	308	ARG	6.9
8	S	42	HIS	6.9
3	N	385	LYS	6.8
1	A	231	GLN	6.8
11	K	107	LYS	6.8
8	S	39	GLY	6.7
1	A	232	THR	6.7
3	C	385	LYS	6.7
1	A	215	LYS	6.6
5	E	46	ASN	6.6
4	D	308	ARG	6.5
11	K	79	GLU	6.5
11	K	80	PRO	6.5
8	S	44	ALA	6.4
5	P	46	ASN	6.4
2	M	332	VAL	6.2
5	P	100	ALA	6.2
11	V	80	PRO	6.2
12	W	9	LYS	6.2
11	V	107	LYS	6.2
6	Q	118	GLU	6.1
6	F	117	LEU	5.9
11	K	42	GLY	5.9
4	O	309	LYS	5.9
6	F	115	ALA	5.9
11	V	24	ARG	5.9
11	K	16	GLY	5.8
1	A	229	SER	5.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	H	38	GLN	5.7
7	R	127	LYS	5.7
1	A	227	ASN	5.7
8	S	37	LEU	5.6
8	H	48	SER	5.6
5	P	45	GLU	5.4
10	U	45	LYS	5.3
6	F	118	GLU	5.3
2	B	211	ALA	5.3
5	E	103	LEU	5.3
12	W	55	ASP	5.2
5	P	213	ILE	5.2
5	P	47	ASN	5.2
5	P	211	LYS	5.1
10	U	66	ASP	5.1
3	N	383	VAL	5.1
10	U	55	VAL	5.1
1	L	28	GLU	5.1
11	V	65	SER	5.0
11	K	75	ILE	5.0
1	L	234	THR	5.0
1	L	125	ILE	4.9
11	K	14	SER	4.9
1	A	381	GLY	4.9
2	B	337	GLU	4.9
2	M	333	SER	4.9
11	V	70	ASP	4.9
10	J	42	PRO	4.9
1	A	130	ASN	4.9
1	L	231	GLN	4.9
10	U	65	LYS	4.8
11	K	24	ARG	4.8
9	T	55	ARG	4.8
2	M	344	LYS	4.8
5	E	49	ALA	4.7
8	S	52	PHE	4.7
10	U	43	GLY	4.7
1	L	29	VAL	4.7
11	V	100	ALA	4.7
4	D	210	PRO	4.6
4	D	309	LYS	4.6
11	K	43	THR	4.6

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Mol	Chain	Res	Type	RSRZ
11	V	83	ILE	4.6
7	G	127	LYS	4.6
11	V	33	LEU	4.6
11	V	103	LYS	4.6
6	F	116	ASP	4.6
1	L	129	ALA	4.5
2	M	329	ASN	4.5
12	W	108	GLU	4.5
5	E	210	ASP	4.5
9	I	56	ILE	4.5
2	B	218	LYS	4.5
1	A	44	PRO	4.5
1	A	28	GLU	4.5
1	L	128	LYS	4.5
10	J	45	LYS	4.5
11	K	40	PRO	4.4
11	V	3	GLU	4.4
6	Q	116	ASP	4.4
10	U	42	PRO	4.4
11	V	7	THR	4.4
1	L	238	LEU	4.4
5	E	45	GLU	4.3
5	P	91	MET	4.3
8	S	43	ASN	4.3
11	V	4	LEU	4.3
8	S	45	VAL	4.3
2	M	339	ASN	4.3
1	A	127	GLN	4.2
4	O	210	PRO	4.2
11	V	18	ARG	4.2
9	T	2	SER	4.2
11	K	10	SER	4.2
1	A	271	ASN	4.2
2	M	211	ALA	4.2
6	Q	115	ALA	4.2
8	H	53	LYS	4.1
6	Q	112	PRO	4.1
11	V	11	LEU	4.1
11	K	70	ASP	4.1
6	F	112	PRO	4.1
5	E	153	LEU	4.0
11	V	60	SER	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
12	W	107	CYS	4.0
11	V	75	ILE	4.0
11	V	35	TRP	4.0
12	W	28	GLY	4.0
1	A	225	SER	4.0
1	L	217	GLU	4.0
2	M	218	LYS	4.0
11	V	105	GLU	4.0
11	V	88	CYS	3.9
5	P	153	LEU	3.9
11	V	9	VAL	3.9
11	K	17	ASP	3.9
3	N	156	PHE	3.9
11	V	86	TYR	3.9
10	U	127	PRO	3.9
1	L	457	TRP	3.9
1	L	130	ASN	3.9
12	W	94	LYS	3.9
2	B	331	SER	3.9
10	J	127	PRO	3.9
5	P	210	ASP	3.8
2	M	341	ASP	3.8
11	K	65	SER	3.8
12	W	49	GLU	3.8
2	M	166	ARG	3.8
1	L	225	SER	3.7
1	A	29	VAL	3.7
10	U	83	LEU	3.7
11	V	17	ASP	3.7
10	J	65	LYS	3.7
1	A	35	GLY	3.7
1	A	30	THR	3.7
11	K	15	LEU	3.7
1	L	44	PRO	3.6
11	V	8	PRO	3.6
12	W	27	LYS	3.6
2	M	318	ILE	3.6
11	V	41	ASP	3.6
8	H	4	PRO	3.6
1	L	233	GLY	3.6
2	B	22	ARG	3.6
5	P	49	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	32	LEU	3.6
1	L	35	GLY	3.6
12	W	50	GLY	3.6
10	U	15	SER	3.5
11	K	29	ILE	3.5
1	L	31	GLN	3.5
11	K	7	THR	3.5
8	S	86	ARG	3.5
11	V	30	ASN	3.5
12	W	42	GLY	3.5
1	L	215	LYS	3.5
1	L	235	LYS	3.5
1	L	32	LEU	3.5
11	V	69	THR	3.5
2	B	266	GLU	3.5
10	U	44	ASN	3.5
4	D	211	GLY	3.5
5	E	100	ALA	3.5
11	K	86	TYR	3.4
11	V	10	SER	3.4
1	L	271	ASN	3.4
11	V	12	ALA	3.4
6	F	74	VAL	3.4
11	K	41	ASP	3.4
11	V	28	ASP	3.4
11	K	23	CYS	3.4
1	A	31	GLN	3.4
5	E	89	LEU	3.4
10	U	31	SER	3.4
1	L	232	THR	3.4
1	A	126	GLN	3.3
7	G	23	LYS	3.3
2	B	330	GLU	3.3
9	T	26	PHE	3.3
5	P	208	ASP	3.3
11	V	34	ASN	3.3
11	V	43	THR	3.3
5	E	91	MET	3.3
1	L	126	GLN	3.3
11	K	73	LEU	3.3
1	L	239	LYS	3.3
11	K	104	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
8	H	68	TYR	3.3
11	K	100	ALA	3.3
2	B	339	ASN	3.2
10	J	43	GLY	3.2
1	A	457	TRP	3.2
11	K	74	THR	3.2
1	A	124	PHE	3.2
11	V	32	PHE	3.2
12	W	4	LYS	3.2
2	B	166	ARG	3.2
11	V	23	CYS	3.2
1	A	241	LYS	3.1
3	C	156	PHE	3.1
1	A	125	ILE	3.1
2	B	213	LYS	3.1
10	U	62	PRO	3.1
1	A	45	SER	3.1
11	K	103	LYS	3.1
11	K	88	CYS	3.1
2	B	17	LEU	3.1
8	S	2	GLY	3.1
10	J	62	PRO	3.1
1	A	233	GLY	3.1
2	B	333	SER	3.1
10	J	76	LYS	3.1
5	P	48	ASP	3.0
11	K	81	GLU	3.0
2	M	238	VAL	3.0
5	P	97	ASN	3.0
11	V	81	GLU	3.0
12	W	26	GLU	3.0
2	B	368	LEU	3.0
11	V	36	TYR	3.0
11	V	104	LEU	3.0
11	K	94	PHE	3.0
11	V	13	ALA	3.0
10	J	125	ARG	3.0
1	L	236	PRO	3.0
1	L	240	LYS	3.0
12	W	59	LYS	3.0
11	V	20	THR	2.9
1	A	219	LEU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	M	250	LEU	2.9
2	M	50	LEU	2.9
1	L	208	VAL	2.9
12	W	21[A]	GLN	2.9
11	K	87	PHE	2.9
6	F	106	LYS	2.9
11	V	73	LEU	2.9
8	H	7	LYS	2.9
8	H	56	PHE	2.9
12	W	5	ALA	2.9
11	K	3	GLU	2.8
11	V	39	LYS	2.8
1	A	240	LYS	2.8
11	V	59	PRO	2.8
12	W	92	LYS	2.8
7	R	20	VAL	2.8
2	B	347	LYS	2.8
9	T	3	PHE	2.8
11	V	94	PHE	2.8
11	K	60	SER	2.8
7	R	23	LYS	2.8
8	S	5	SER	2.8
11	V	89	GLN	2.8
11	V	74	THR	2.8
2	B	335	PRO	2.8
11	V	26	SER	2.8
2	B	50	LEU	2.7
10	U	81	LEU	2.7
4	D	286	TRP	2.7
1	A	235	LYS	2.7
8	H	86	ARG	2.7
6	Q	103	GLU	2.7
8	S	7	LYS	2.7
11	V	21	ILE	2.7
7	G	19	PRO	2.7
12	W	13	THR	2.7
2	B	238	VAL	2.7
2	M	266	GLU	2.7
11	K	77	ASN	2.7
8	H	87	GLU	2.7
1	A	122	GLN	2.6
7	G	17	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
12	W	56	ALA	2.6
10	J	1	GLU	2.6
12	W	30	PRO	2.6
11	V	63	SER	2.6
1	A	111	GLY	2.6
2	B	33	VAL	2.6
8	H	50	ARG	2.6
2	B	217	SER	2.6
10	J	89	GLU	2.6
10	U	1	GLU	2.6
1	L	30	THR	2.6
2	B	256	LEU	2.6
1	A	226	LYS	2.6
2	M	328	GLN	2.6
11	V	19	VAL	2.6
7	G	90	ARG	2.5
11	K	33	LEU	2.5
5	P	102	PRO	2.5
7	R	19	PRO	2.5
12	W	105	LYS	2.5
5	P	99	ALA	2.5
12	W	81	PRO	2.5
6	Q	74	VAL	2.5
10	J	55	VAL	2.5
10	U	103	SER	2.5
2	M	248	ALA	2.5
2	M	31	LEU	2.5
5	E	40	ASP	2.5
8	H	2	GLY	2.5
9	I	3	PHE	2.5
5	P	124	HIS	2.5
6	F	114	TYR	2.5
1	L	228	LEU	2.5
6	Q	114	TYR	2.5
1	A	221	ASN	2.5
1	A	115	LYS	2.4
5	P	154	ILE	2.4
5	E	97	ASN	2.4
10	U	122	SER	2.4
11	K	13	ALA	2.4
11	V	2	ILE	2.4
10	J	83	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
10	U	68	LEU	2.4
5	P	123	PRO	2.4
10	J	3	LYS	2.4
2	B	220	GLU	2.4
9	I	9	THR	2.4
6	F	97	HIS	2.4
2	M	256	LEU	2.4
2	M	219	SER	2.4
11	V	67	SER	2.4
10	J	57	ASP	2.4
2	B	318	ILE	2.4
6	F	113	GLY	2.4
1	L	122	GLN	2.4
1	A	238	LEU	2.4
9	I	26	PHE	2.4
1	A	114	ASP	2.4
1	A	118	ASP	2.4
1	A	218	ASP	2.4
11	V	61	ARG	2.4
2	M	292	GLN	2.4
5	P	212	VAL	2.4
11	K	2	ILE	2.4
10	J	66	ASP	2.3
11	K	76	SER	2.3
12	W	8	ALA	2.3
11	K	32	PHE	2.3
11	V	87	PHE	2.3
4	D	209	PRO	2.3
1	L	45	SER	2.3
1	L	72	LEU	2.3
4	O	137	GLU	2.3
1	L	237	VAL	2.3
10	J	49	VAL	2.3
4	D	307	PRO	2.3
4	O	307	PRO	2.3
12	W	3	PHE	2.3
11	V	40	PRO	2.3
11	V	102	THR	2.3
7	R	126	SER	2.3
5	P	31	LYS	2.3
2	B	343	VAL	2.3
11	K	89	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	401	LEU	2.3
2	M	17	LEU	2.3
5	P	105	LYS	2.3
6	Q	110	GLN	2.2
1	A	34	ASN	2.2
2	M	213	LYS	2.2
10	U	88	THR	2.2
11	V	97	THR	2.2
5	E	118	ILE	2.2
11	V	76	SER	2.2
5	P	103	LEU	2.2
10	J	81	LEU	2.2
11	K	4	LEU	2.2
1	L	381	GLY	2.2
1	A	217	GLU	2.2
2	M	187	VAL	2.2
6	Q	113	GLY	2.2
2	M	22	ARG	2.2
11	V	51	THR	2.2
2	M	327	VAL	2.2
11	K	83	ILE	2.2
2	B	345	ASP	2.2
12	W	29	GLY	2.2
10	J	44	ASN	2.2
1	L	401	LEU	2.2
6	F	110	GLN	2.2
11	V	99	GLY	2.2
4	D	62	MET	2.1
6	Q	117	LEU	2.1
7	G	10	ARG	2.1
11	K	22	SER	2.1
2	M	25	PRO	2.1
11	K	8	PRO	2.1
8	H	91	ARG	2.1
10	U	3	LYS	2.1
11	V	57	GLY	2.1
12	W	6	GLY	2.1
8	S	68	TYR	2.1
11	K	18	ARG	2.1
8	S	56	PHE	2.1
10	J	8	GLY	2.1
4	O	141	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
6	Q	75	THR	2.1
1	A	224	GLU	2.1
1	A	278	ALA	2.1
2	B	310	LYS	2.1
2	M	310	LYS	2.1
2	M	334	SER	2.1
11	V	22	SER	2.1
4	D	135	ASP	2.1
8	S	67	TRP	2.1
12	W	99	LEU	2.1
2	M	345	ASP	2.1
4	D	200	ASP	2.1
5	P	145	ASP	2.1
8	H	67	TRP	2.1
2	M	239	ALA	2.1
1	L	219	LEU	2.1
11	K	54	LEU	2.1
11	K	39	LYS	2.1
7	R	90	ARG	2.0
10	U	125	ARG	2.0
4	D	185	HIS	2.0
11	K	63	SER	2.0
2	M	335	PRO	2.0
1	L	111	GLY	2.0
1	A	36	ILE	2.0
6	Q	130	LEU	2.0
9	T	56	ILE	2.0
11	V	1	ASP	2.0
10	J	74	THR	2.0
1	A	134	SER	2.0
10	U	49	VAL	2.0
2	M	340	PHE	2.0
4	O	239	GLY	2.0
8	S	90	GLU	2.0
11	K	12	ALA	2.0
7	G	97	GLN	2.0
10	U	16	GLN	2.0
2	B	246	ASN	2.0
5	E	213	ILE	2.0
11	V	44	ILE	2.0
1	A	397	LYS	2.0
2	M	220	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

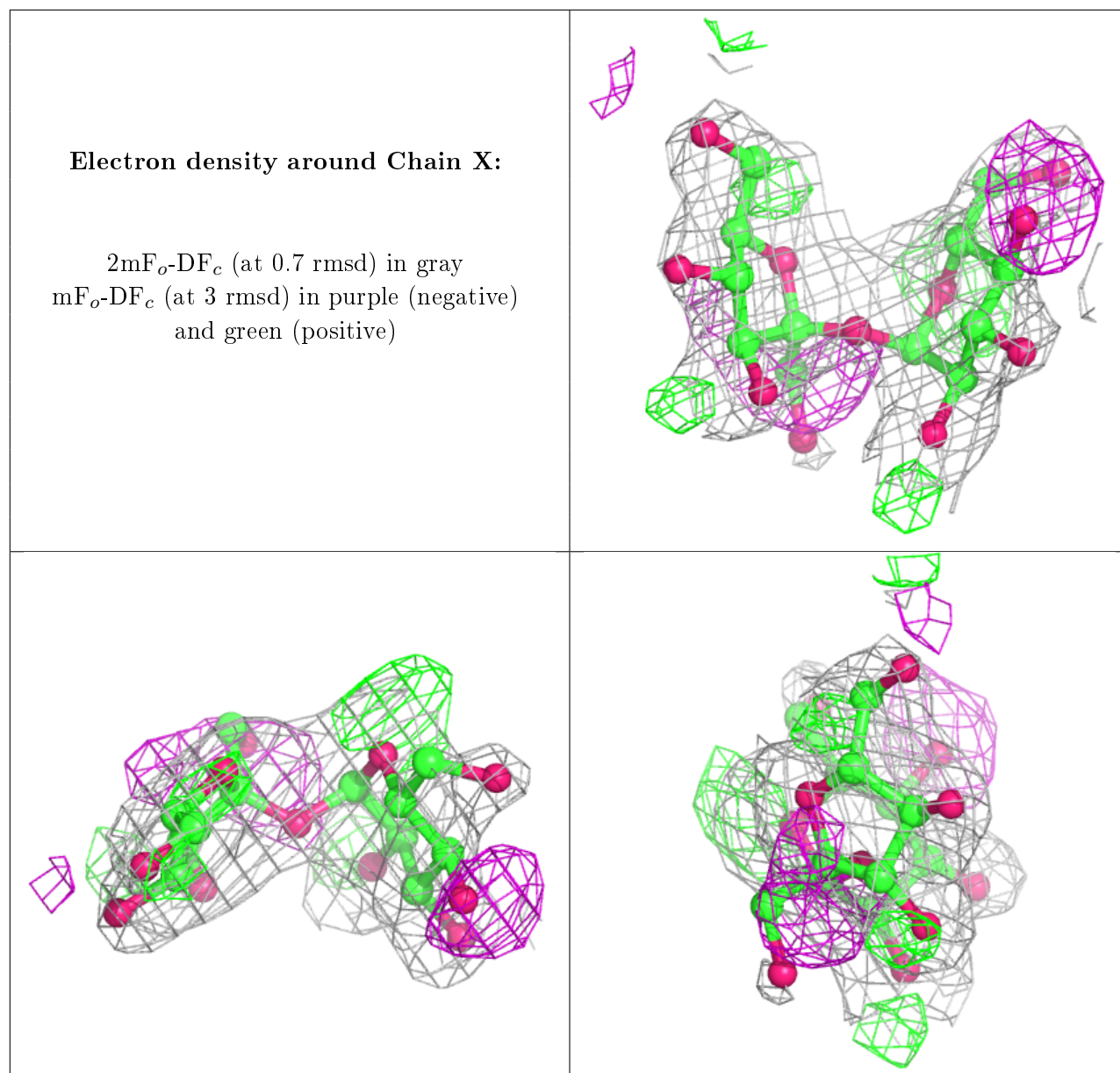
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	M3L	W	77	12/13	0.86	0.32	64,68,72,72	0

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
13	FRU	X	2	12/12	0.69	0.27	68,69,72,72	0
13	GLC	X	1	11/12	0.79	0.20	70,71,73,76	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.



## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
20	CN5	C	4033	41/41	0.63	0.23	76,79,85,86	0
18	8PE	C	4010	47/47	0.81	0.16	39,50,59,60	0
18	8PE	N	4110	47/47	0.82	0.16	43,51,65,67	0
22	CN3	D	4031	55/55	0.86	0.18	48,62,70,71	0

*Continued on next page...*

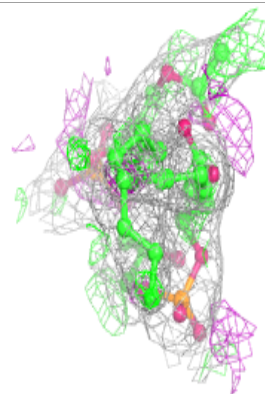
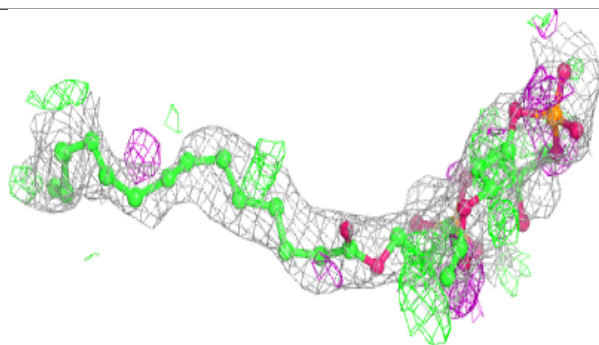
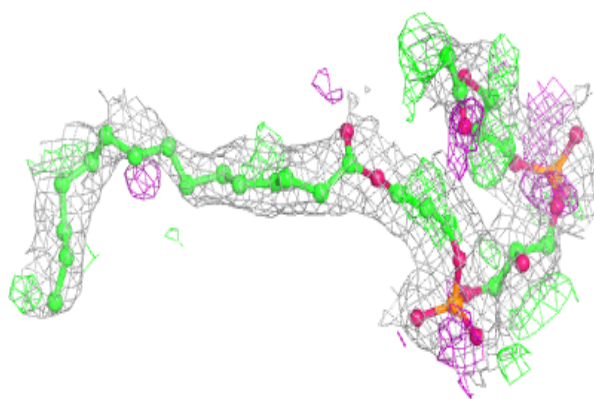
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	6PH	L	4113	40/40	0.86	0.14	51,55,67,68	0
14	6PH	A	4013	40/40	0.89	0.13	48,55,61,61	0
22	CN3	N	4131	55/55	0.90	0.16	39,58,66,69	0
19	9PE	N	4111	40/40	0.91	0.13	39,47,62,66	0
16	HEM	W	4026	43/43	0.92	0.15	46,50,54,55	0
19	9PE	C	4011	40/40	0.93	0.13	39,46,70,72	0
15	UMQ	L	4121	34/34	0.94	0.10	33,35,57,58	0
21	7PH	D	4014	38/38	0.94	0.16	43,46,62,63	0
21	7PH	O	4114	38/38	0.94	0.15	40,44,52,52	0
15	UMQ	A	4021	34/34	0.94	0.11	32,36,55,56	0
17	SMA	N	4025	37/37	0.95	0.11	21,24,30,33	0
17	SMA	C	4005	37/37	0.95	0.11	22,24,31,34	0
16	HEM	D	4003	43/43	0.97	0.12	23,29,33,34	0
16	HEM	N	4022	43/43	0.98	0.10	15,18,26,28	0
16	HEM	N	4021	43/43	0.98	0.08	16,20,25,27	0
16	HEM	O	4023	43/43	0.98	0.09	25,28,30,33	0
16	HEM	C	4002	43/43	0.99	0.08	17,20,24,28	0
23	FES	P	4024	4/4	0.99	0.09	28,29,31,32	0
23	FES	E	4004	4/4	0.99	0.08	27,27,28,31	0
16	HEM	C	4001	43/43	0.99	0.09	16,21,26,30	0

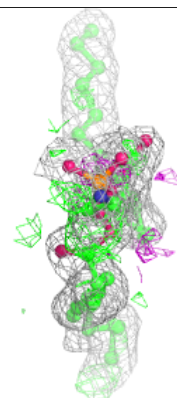
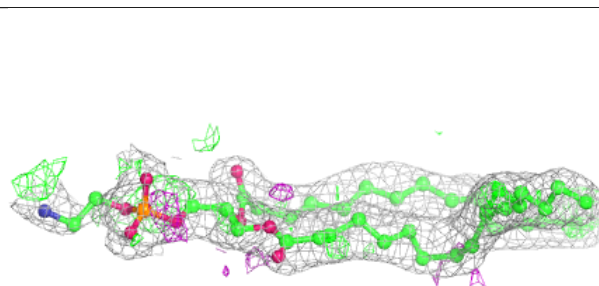
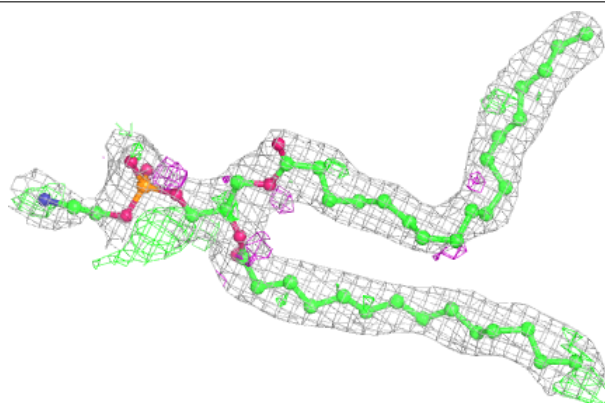
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CN5 C 4033:**

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

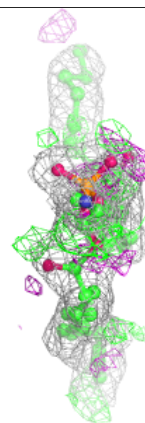
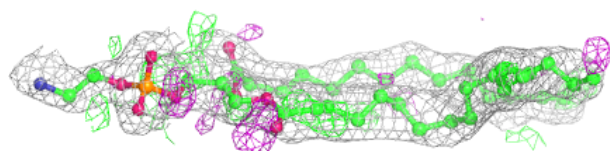
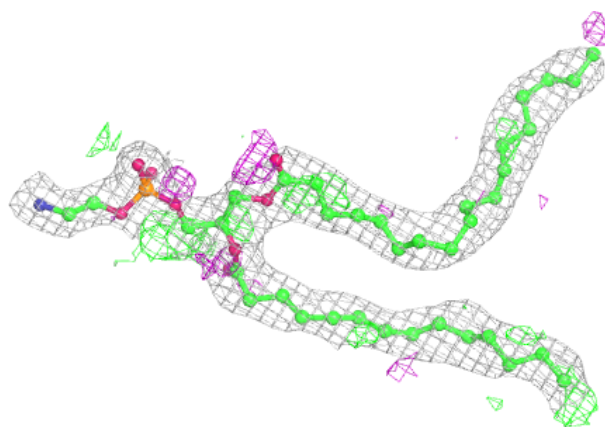
**Electron density around 8PE C 4010:**

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

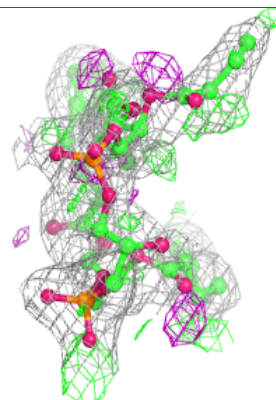
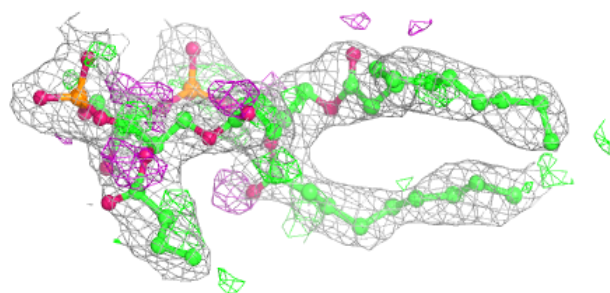
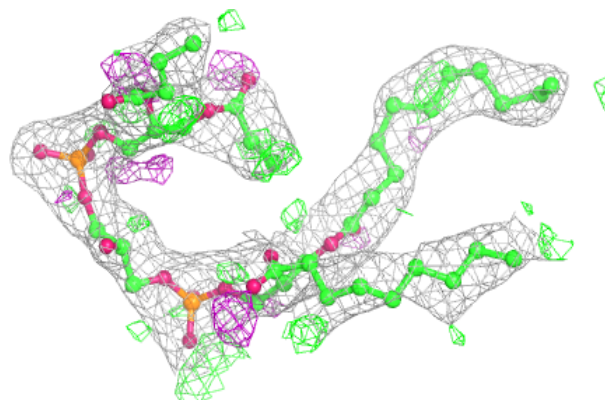


**Electron density around 8PE N 4110:**

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

**Electron density around CN3 D 4031:**

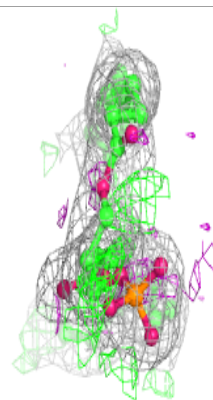
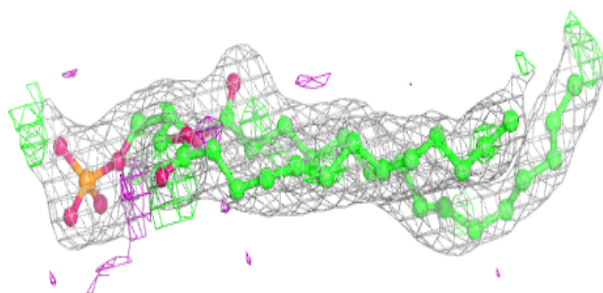
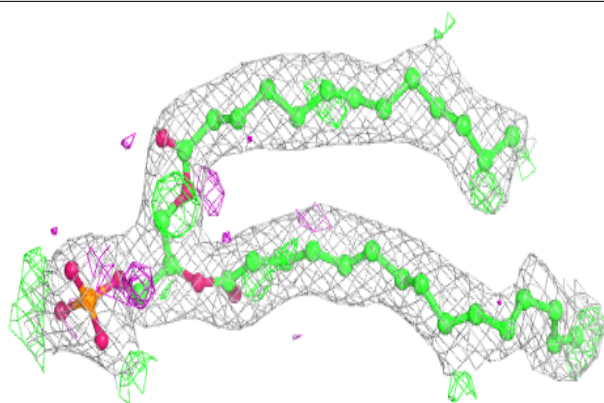
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



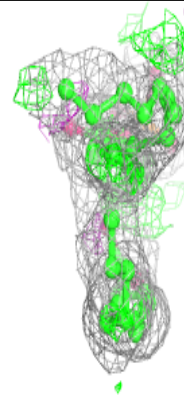
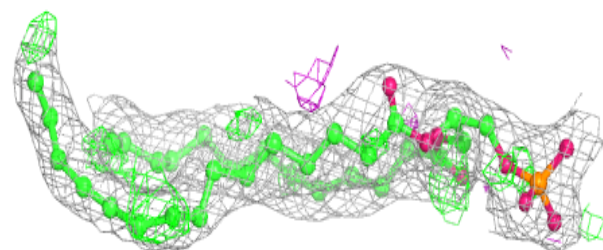
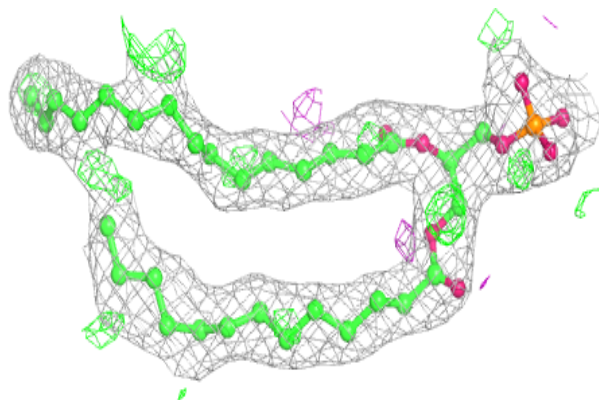


**Electron density around 6PH L 4113:**

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

**Electron density around 6PH A 4013:**

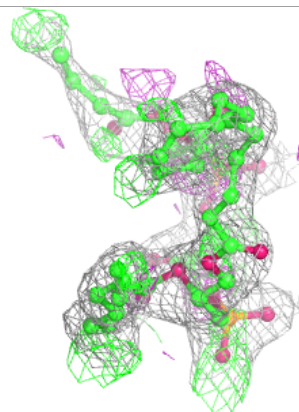
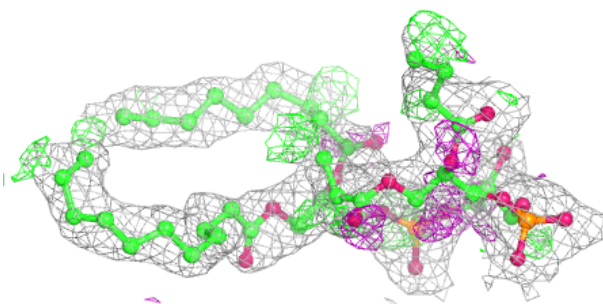
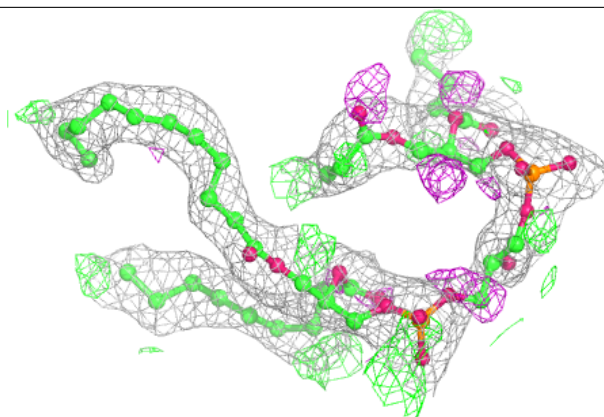
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



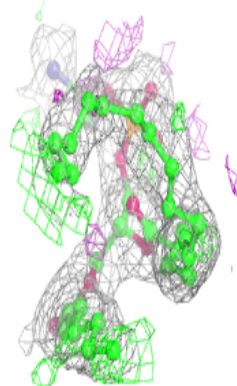
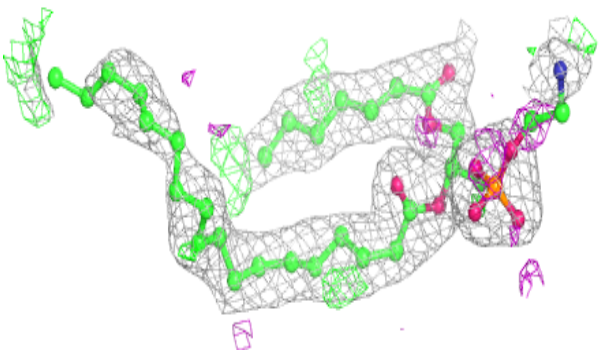
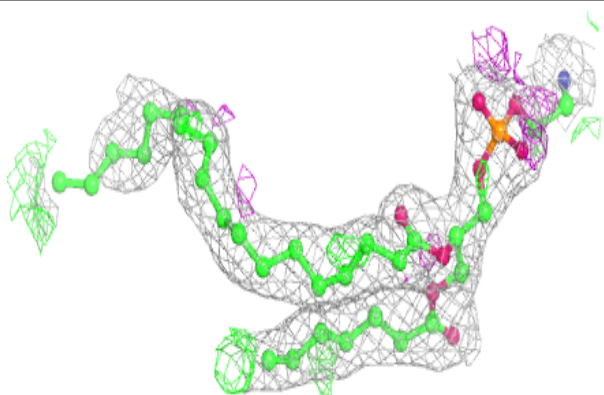


**Electron density around CN3 N 4131:**

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

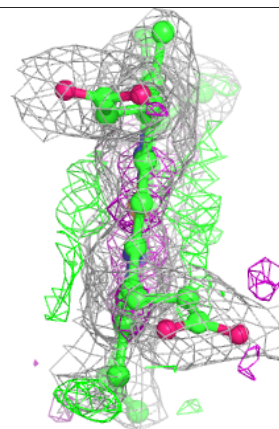
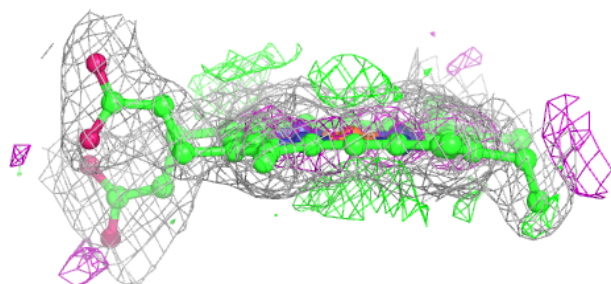
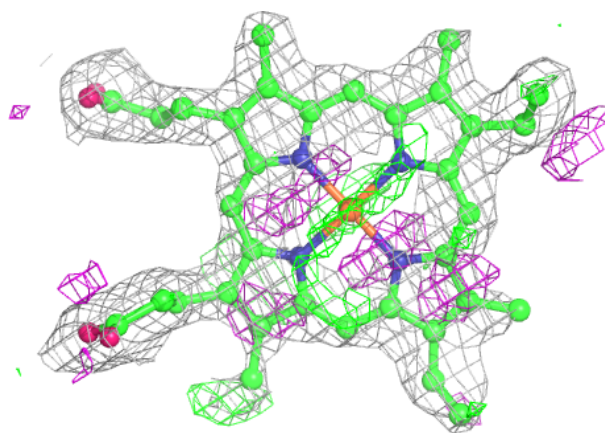
**Electron density around 9PE N 4111:**

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

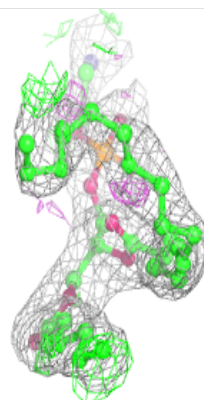
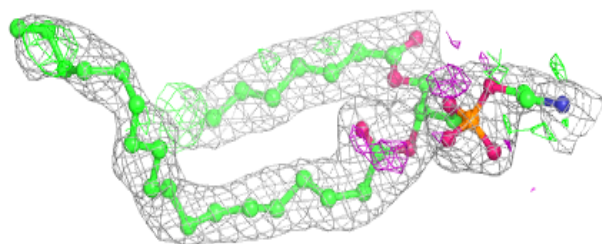
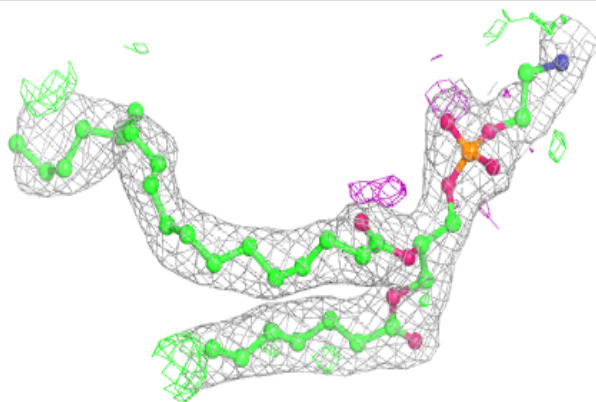


**Electron density around HEM W 4026:**

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

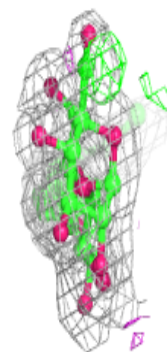
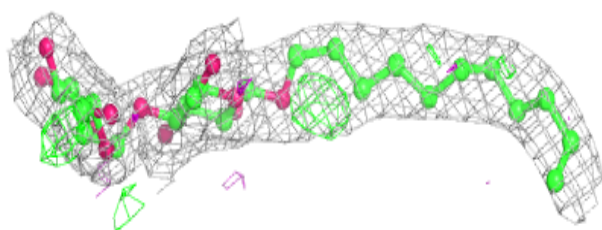
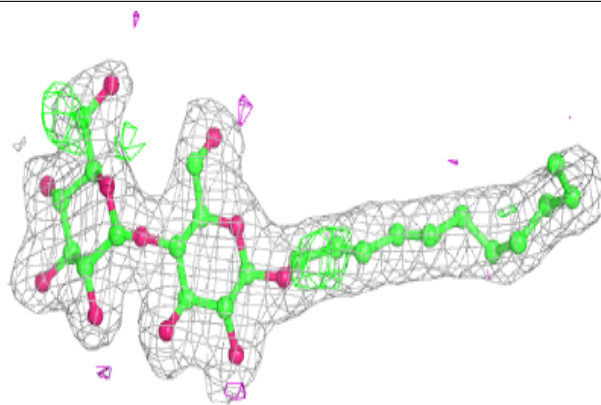
**Electron density around 9PE C 4011:**

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

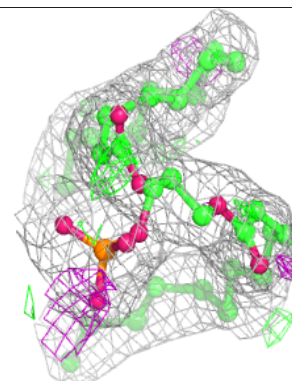
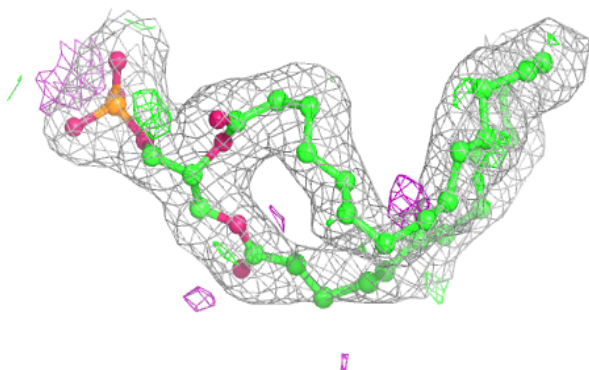
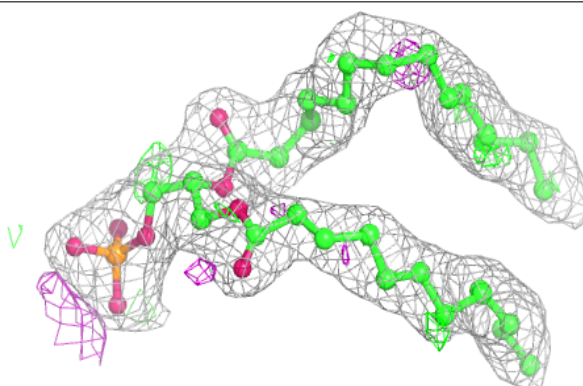


**Electron density around UMQ L 4121:**

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

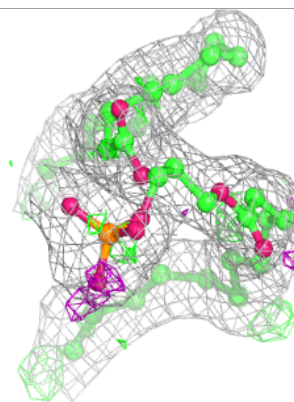
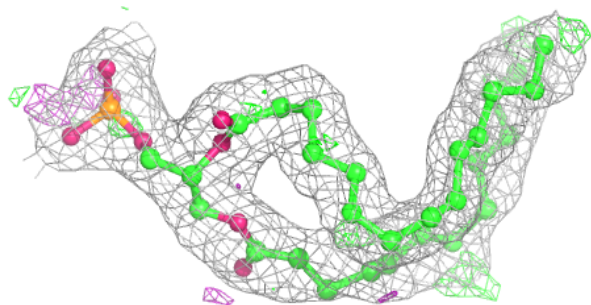
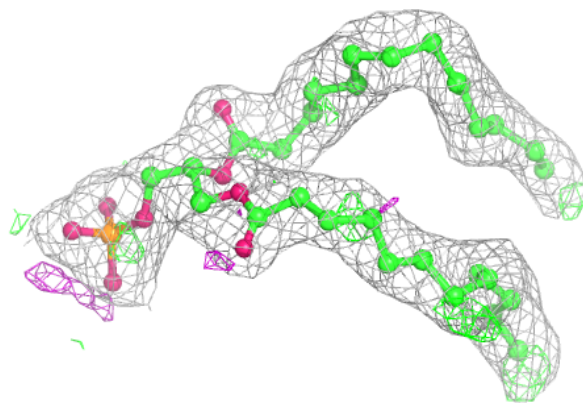
**Electron density around 7PH D 4014:**

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

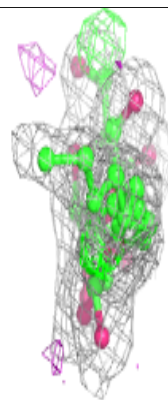
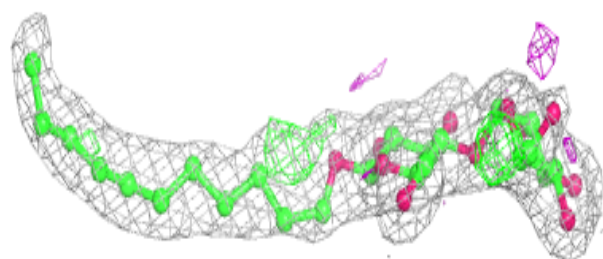
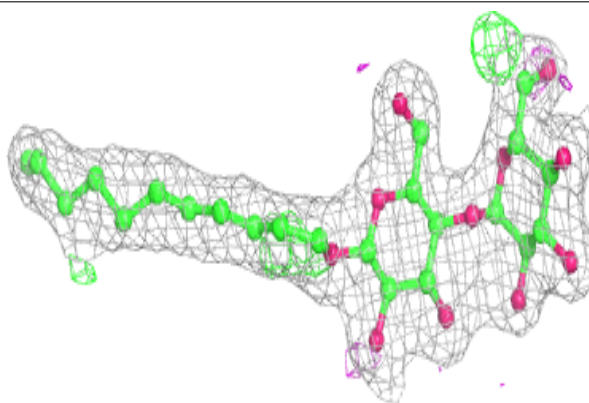


**Electron density around 7PH O 4114:**

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

**Electron density around UMQ A 4021:**

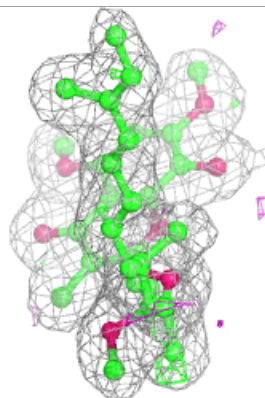
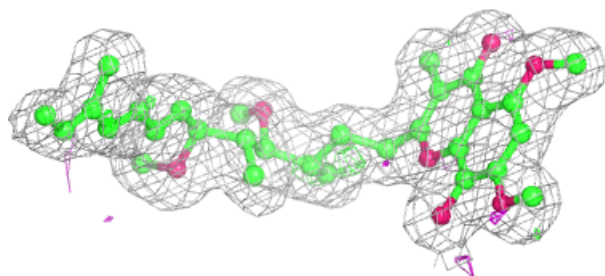
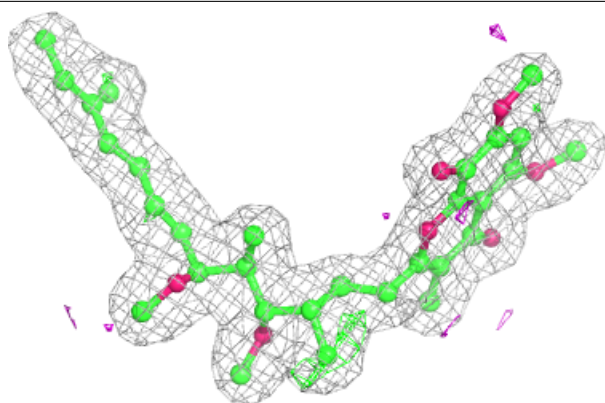
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



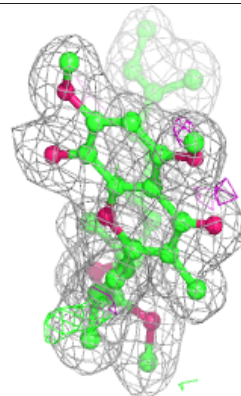
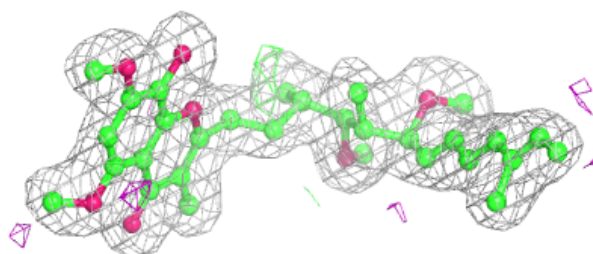
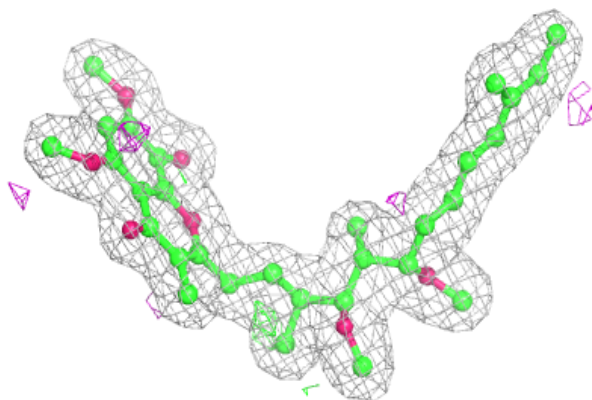


**Electron density around SMA N 4025:**

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

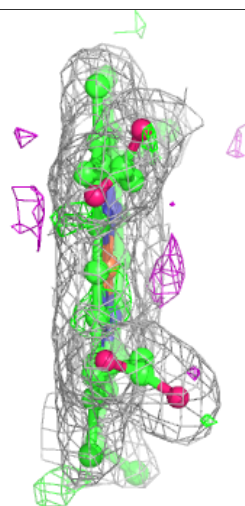
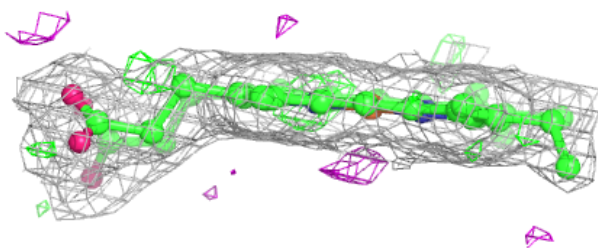
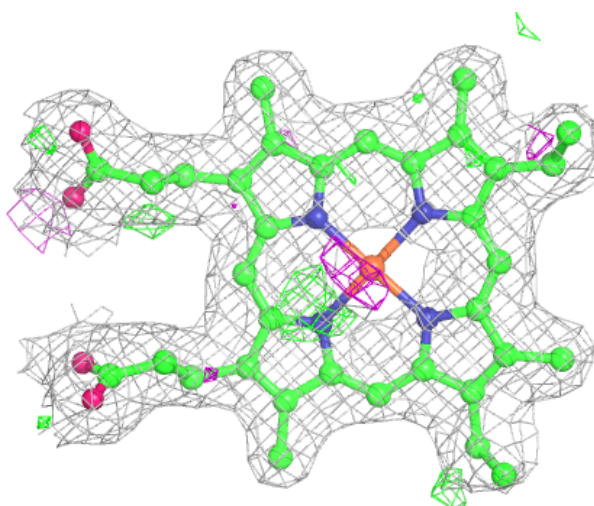
**Electron density around SMA C 4005:**

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



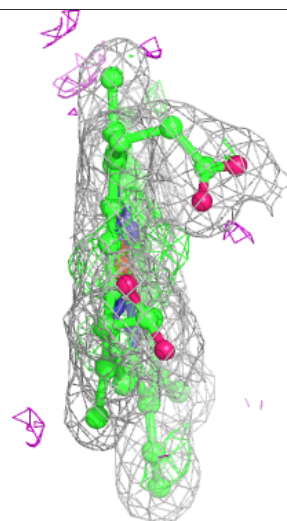
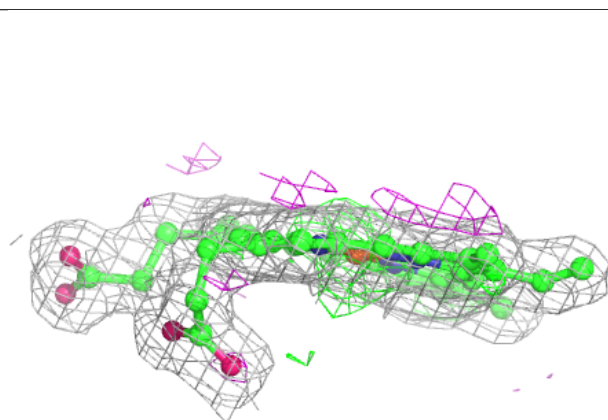
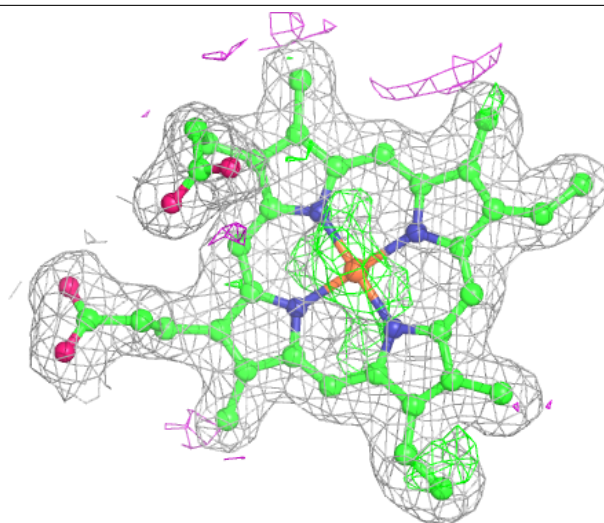
**Electron density around HEM D 4003:**

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



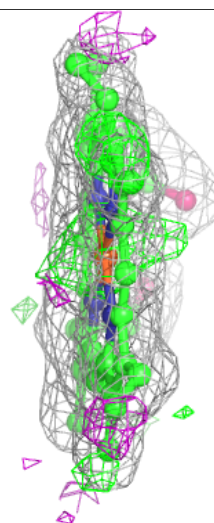
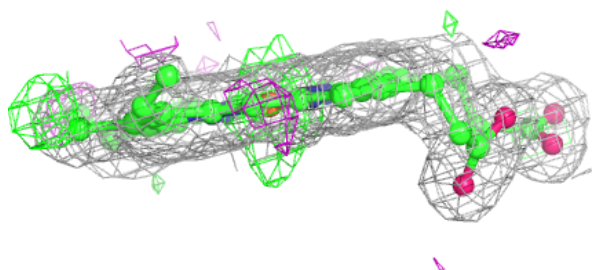
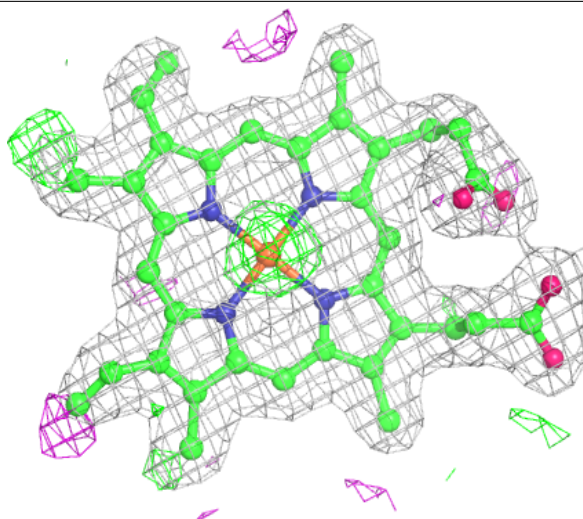
**Electron density around HEM N 4022:**

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



**Electron density around HEM N 4021:**

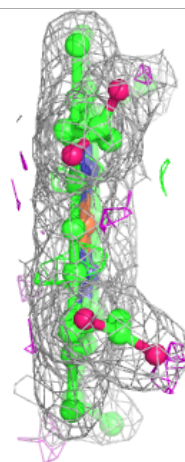
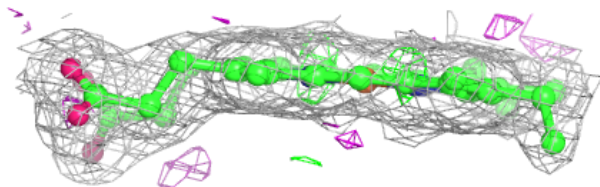
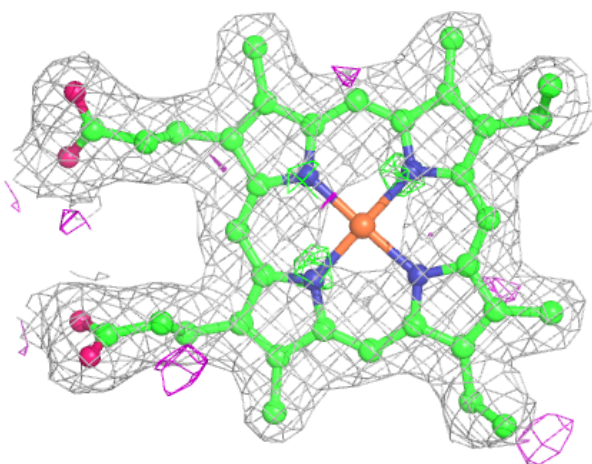
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





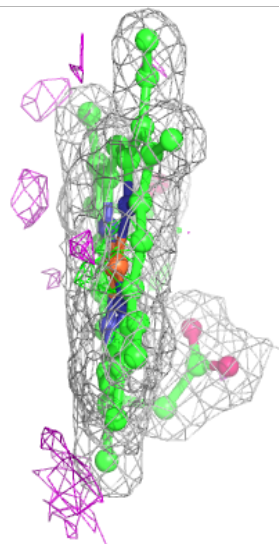
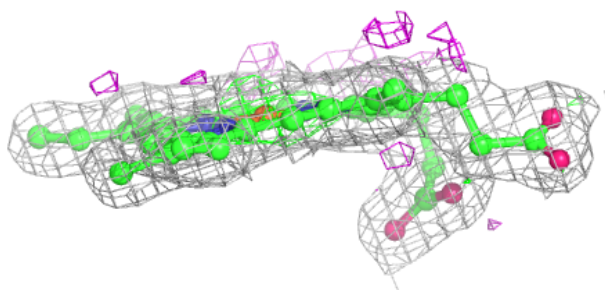
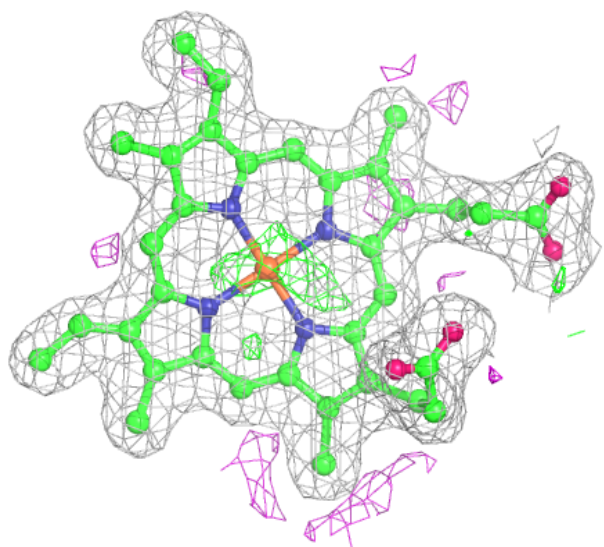
**Electron density around HEM O 4023:**

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



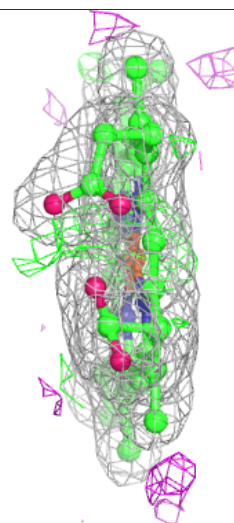
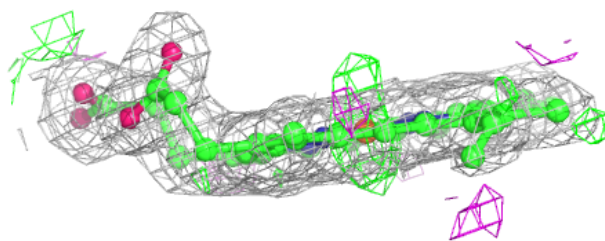
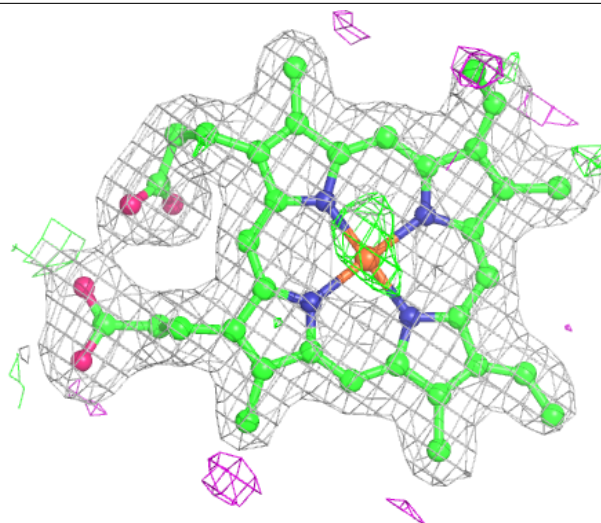
**Electron density around HEM C 4002:**

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



**Electron density around HEM C 4001:**

$2mF_o-DF_c$  (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.