



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 12:27 AM EDT

PDB ID : 3CXH / pdb_00003cxh
Title : Structure of yeast complex III with isoform-2 cytochrome c bound and definition of a minimal core interface for electron transfer.
Authors : Solmaz, S.R.N.; Hunte, C.
Deposited on : 2008-04-24
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

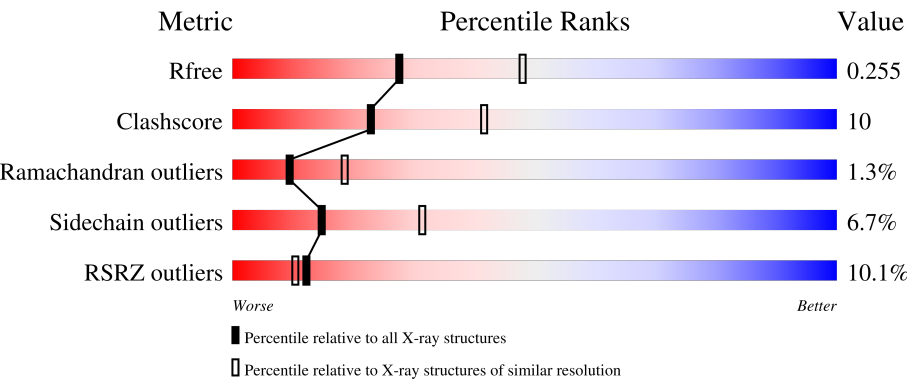
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	431	12% 67%28%5%•
1	L	431	12% 74%22%•
2	B	352	11% 66%28%6%•
2	M	352	10% 67%25%8%
3	C	385	2% 78%19%••

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Mol	Chain	Length	Quality of chain
3	N	385	
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	112	
13	X	2	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 36805 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	246	Total	C	N	O	S	0	0	0
			1940	1237	334	360	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	O	246	Total	C	N	O	S	0	0	0
			1940	1237	334	360	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	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			
7	R	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	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	55	Total	C	N	O	0	0	0
			448	298	75	75			
9	T	55	Total	C	N	O	0	0	0
			448	298	75	75			

- 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			

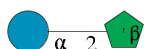
- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

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-2.

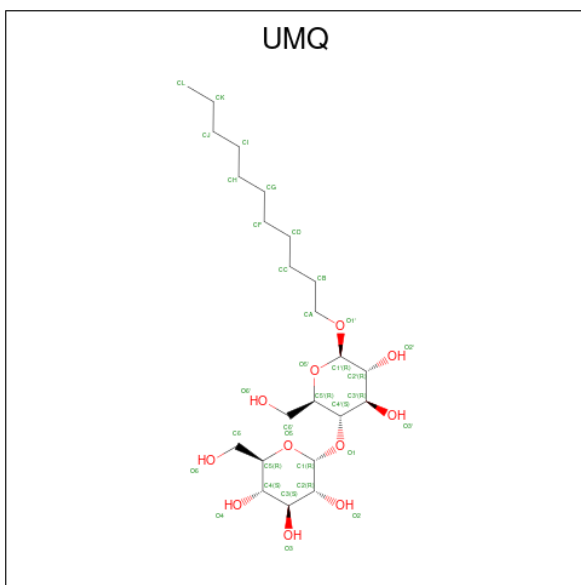
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	112	Total	C	N	O	S	0	1	0
			885	555	159	166	5			

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



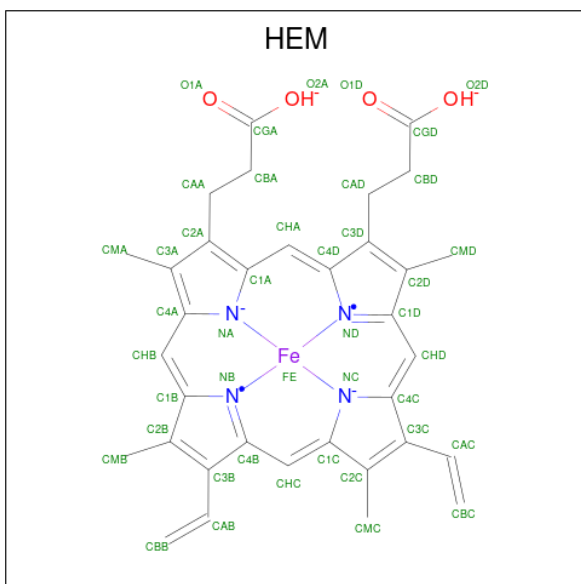
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
13	X	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 14 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



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

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



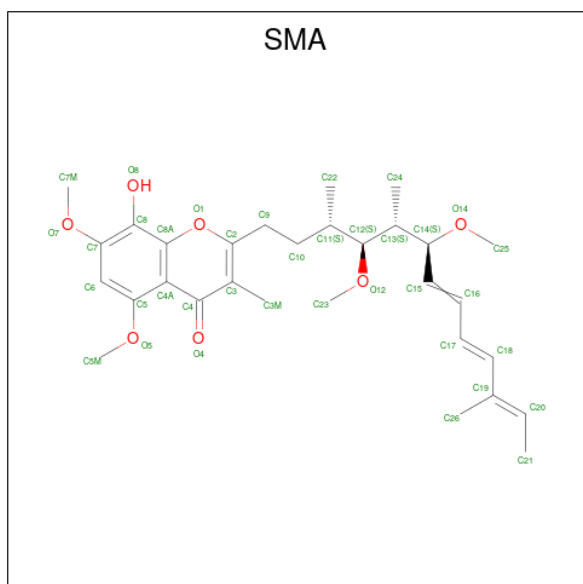
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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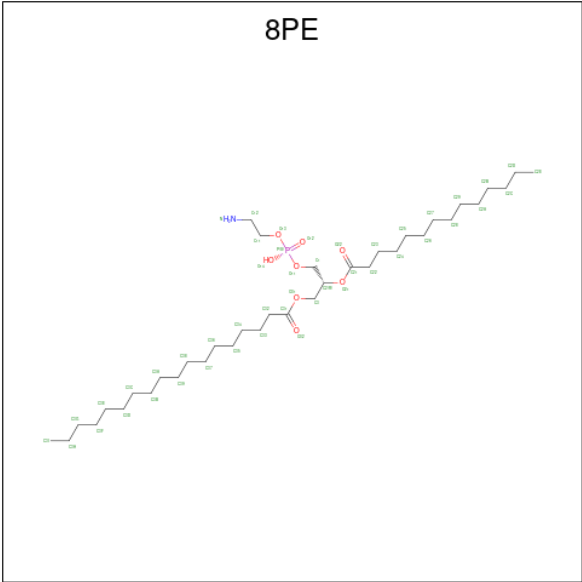
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 16 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



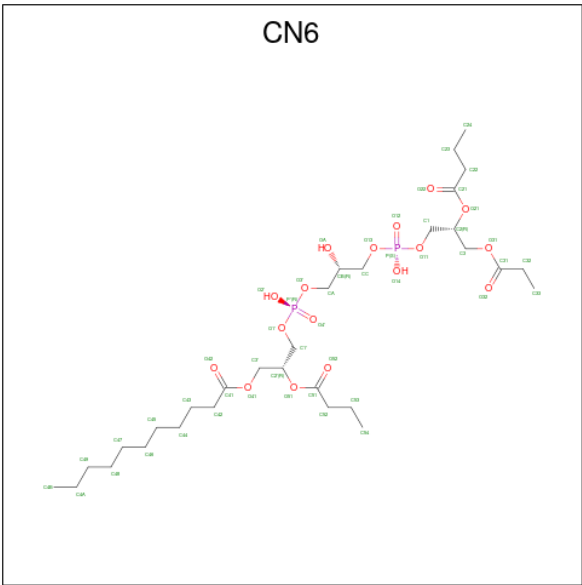
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			37	30	7		
16	N	1	Total	C	O	0	0
			37	30	7		

- Molecule 17 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: $C_{37}H_{74}NO_8P$).



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

- Molecule 18 is (2R,5R,11S,14R)-2-(butanoyloxy)-5,8,11-trihydroxy-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanadec-1-yl undecanoate (CCD ID: CN6) (formula: C₃₁H₅₈O₁₇P₂).



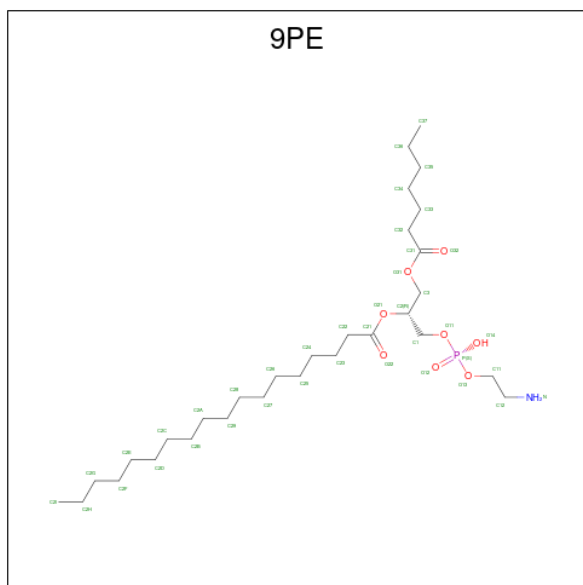
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	C	1	Total	C	O	P	0	0
			50	31	17	2		

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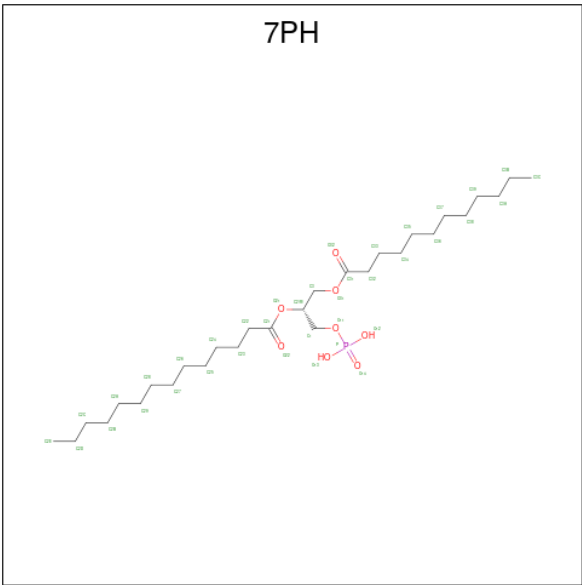
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	N	1	Total	C	O	P	0	0
			50	31	17	2		

- Molecule 19 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: C₃₀H₆₀NO₈P).



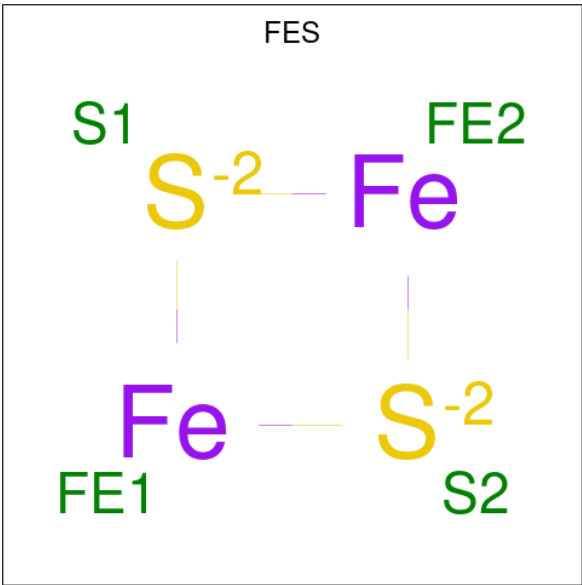
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
19	N	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 20 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).



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

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- # 6PH

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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 23 | A | 42 | Total O
42 42 | 0 | 0 |
| 23 | B | 17 | Total O
17 17 | 0 | 0 |
| 23 | C | 75 | Total O
75 75 | 0 | 0 |
| 23 | D | 50 | Total O
50 50 | 0 | 0 |
| 23 | E | 19 | Total O
19 19 | 0 | 0 |
| 23 | F | 3 | Total O
3 3 | 0 | 0 |
| 23 | G | 21 | Total O
21 21 | 0 | 0 |
| 23 | H | 10 | Total O
10 10 | 0 | 0 |



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	I	4	Total O 4 4	0	0
23	J	2	Total O 2 2	0	0
23	K	1	Total O 1 1	0	0
23	L	54	Total O 54 54	0	0
23	M	15	Total O 15 15	0	0
23	N	88	Total O 88 88	0	0
23	O	74	Total O 74 74	0	0
23	P	18	Total O 18 18	0	0
23	Q	3	Total O 3 3	0	0
23	R	22	Total O 22 22	0	0
23	S	13	Total O 13 13	0	0
23	T	5	Total O 5 5	0	0
23	U	2	Total O 2 2	0	0
23	W	10	Total O 10 10	0	0

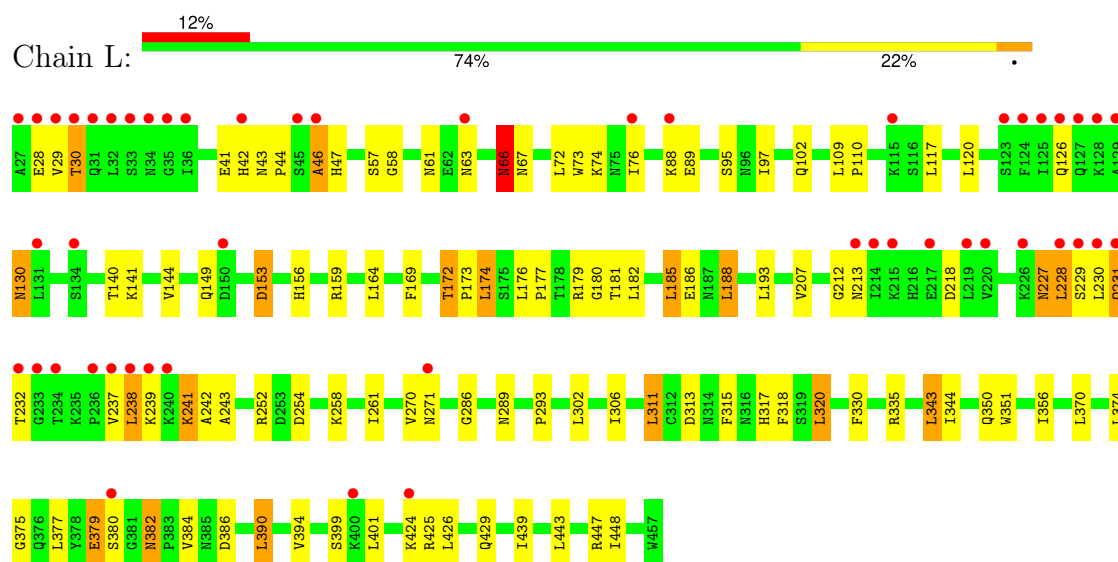
3 Residue-property plots

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.

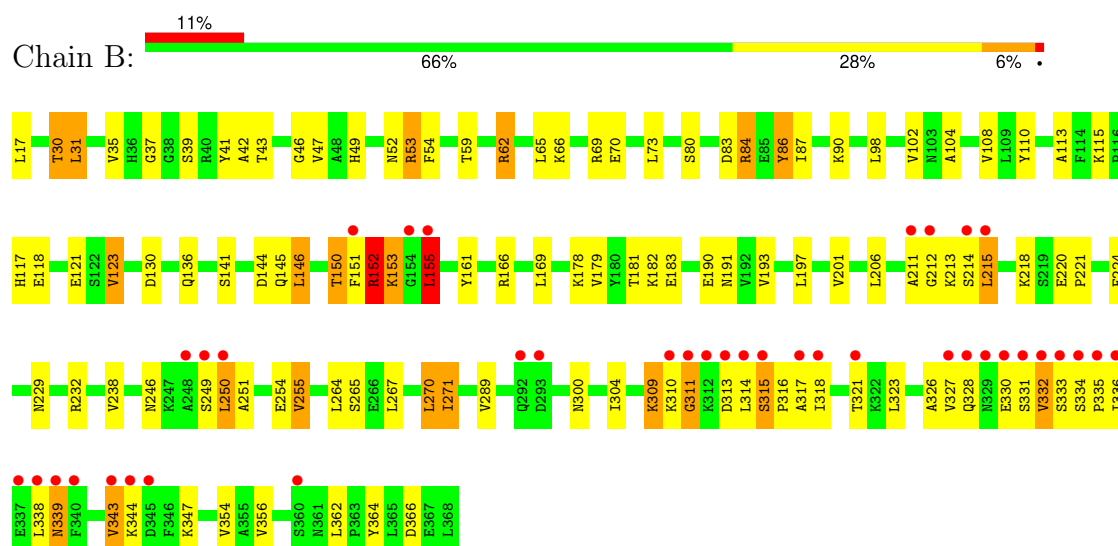
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



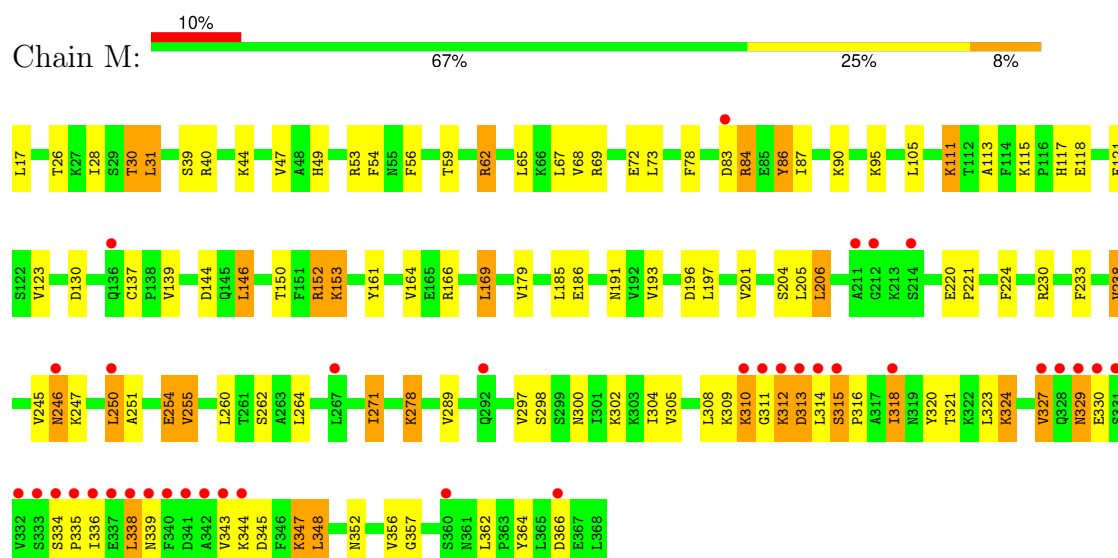
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



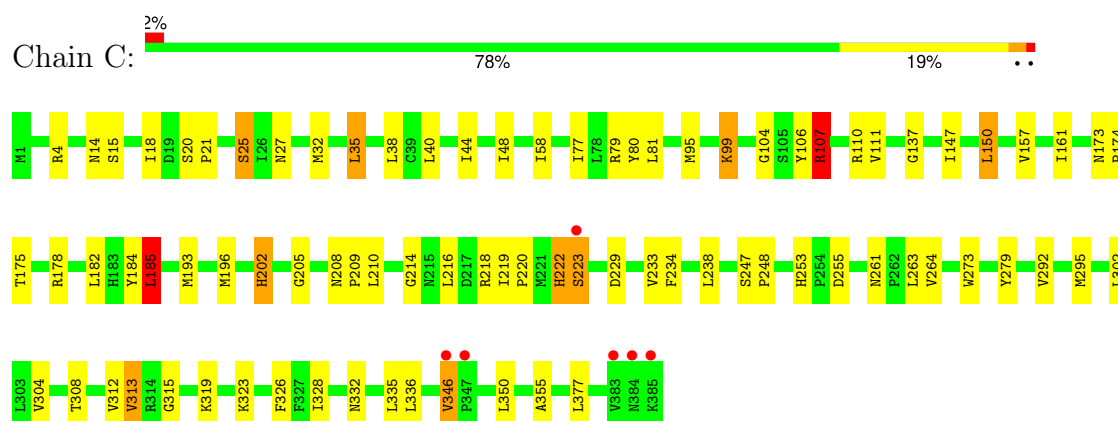
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



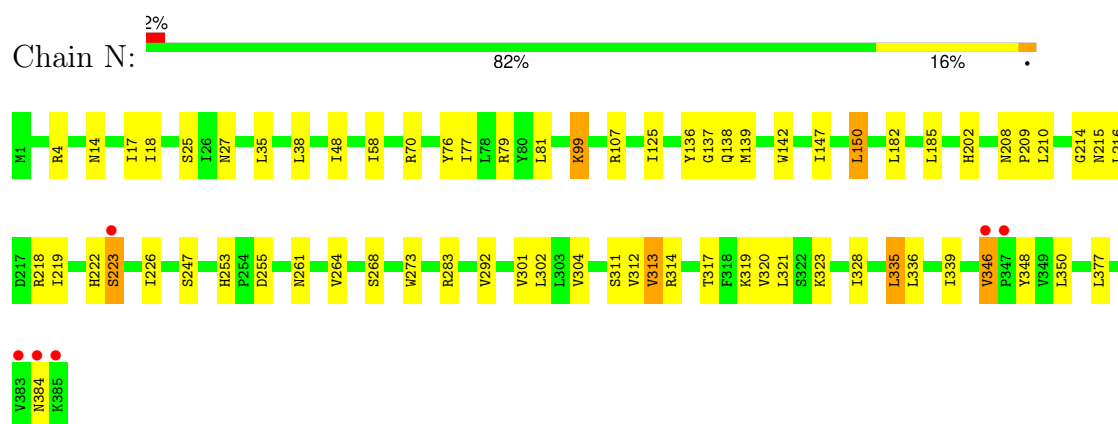
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



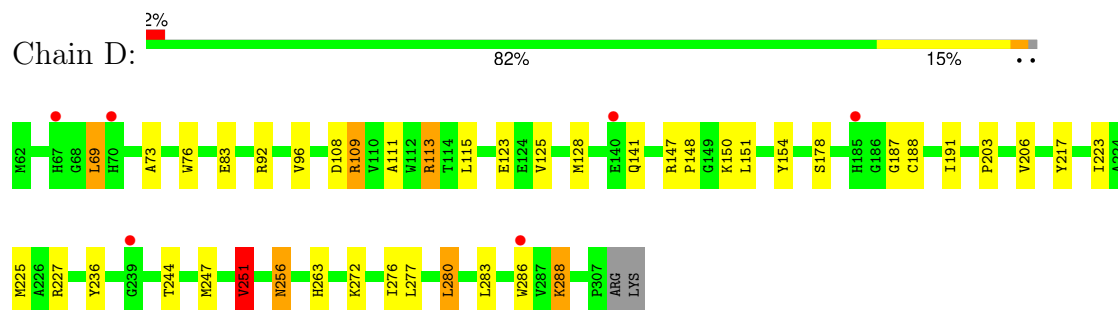
- Molecule 3: Cytochrome b



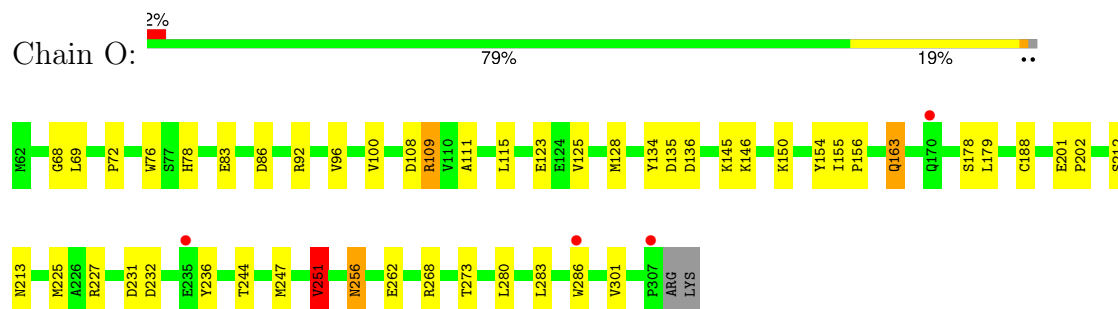
- Molecule 3: Cytochrome b



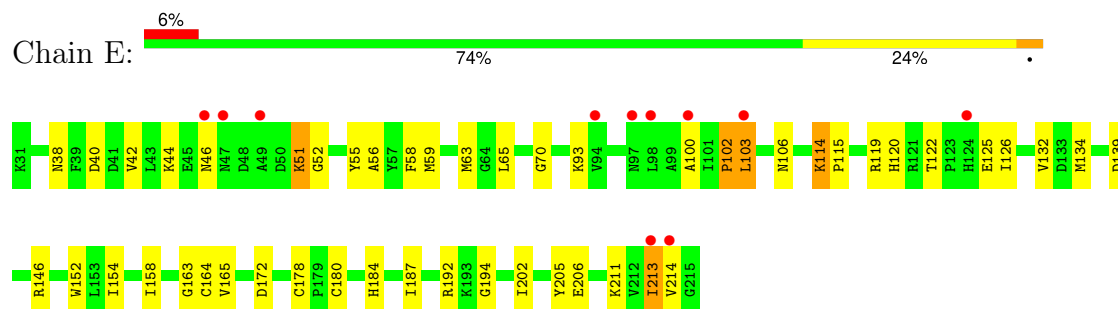
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



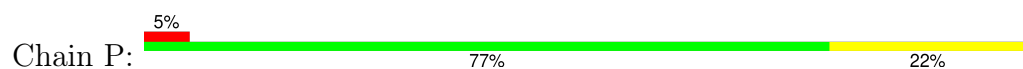
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



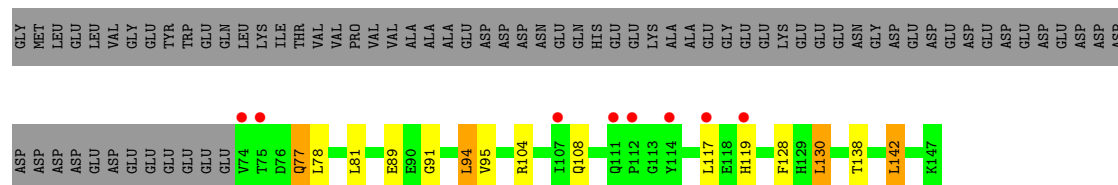
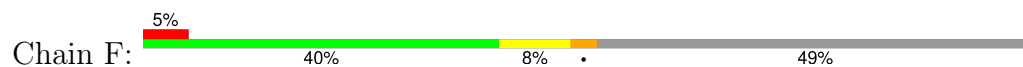
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



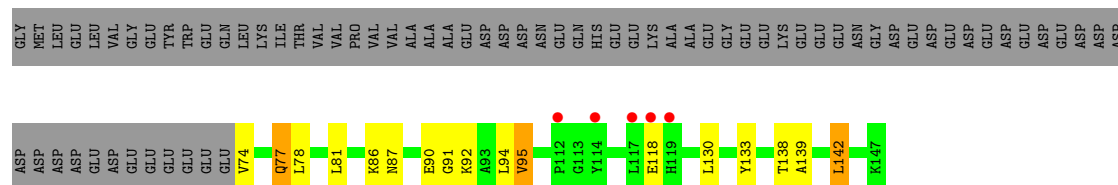
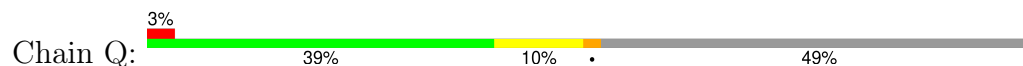
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



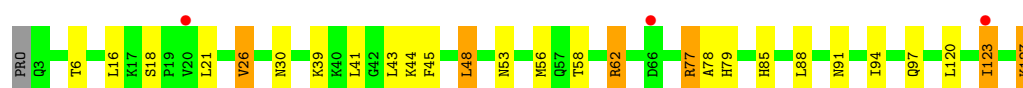
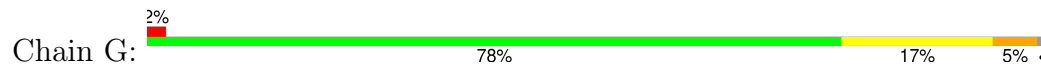
- Molecule 6: Cytochrome b-c1 complex subunit 6



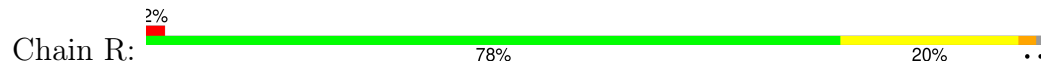
- Molecule 6: Cytochrome b-c1 complex subunit 6



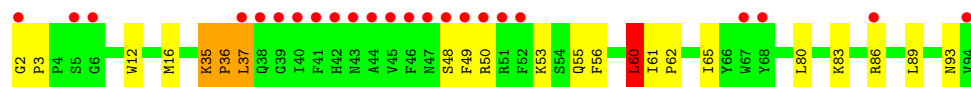
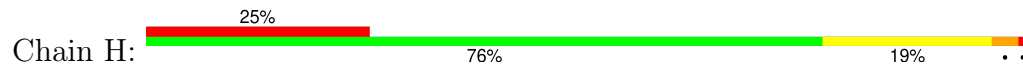
- Molecule 7: Cytochrome b-c1 complex subunit 7



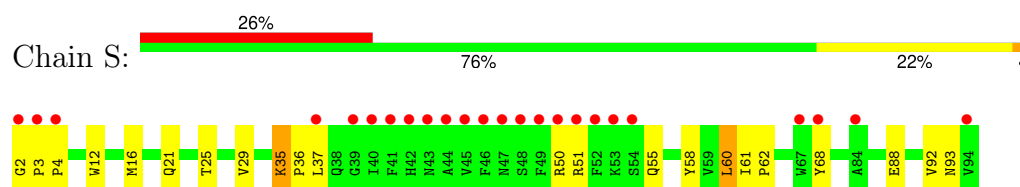
- Molecule 7: Cytochrome b-c1 complex subunit 7



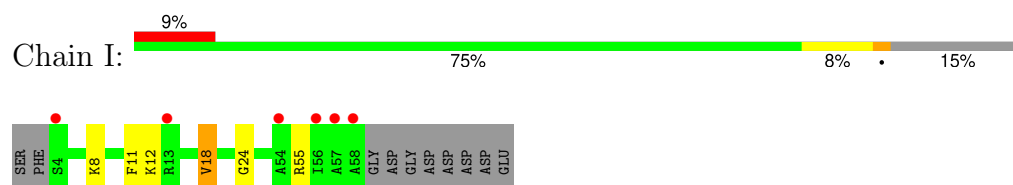
- Molecule 8: Cytochrome b-c1 complex subunit 8



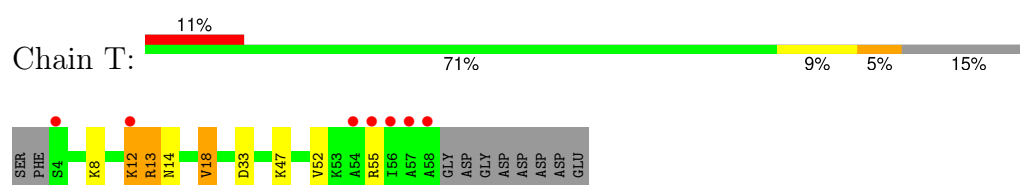
- Molecule 8: Cytochrome b-c1 complex subunit 8



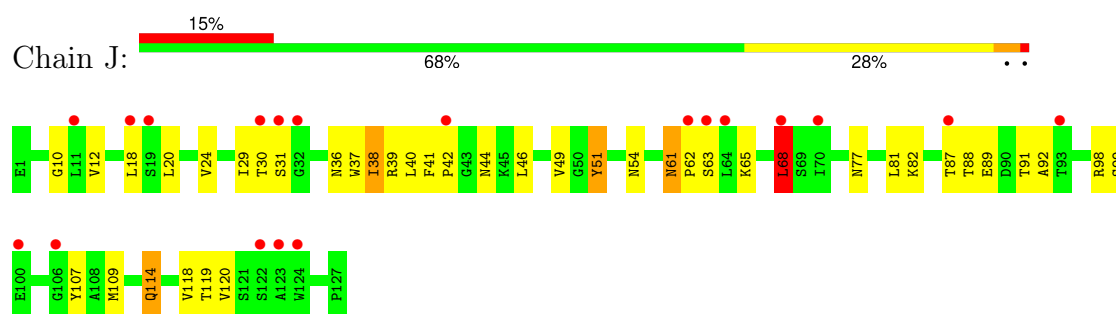
• Molecule 9: Cytochrome b-c1 complex subunit 9



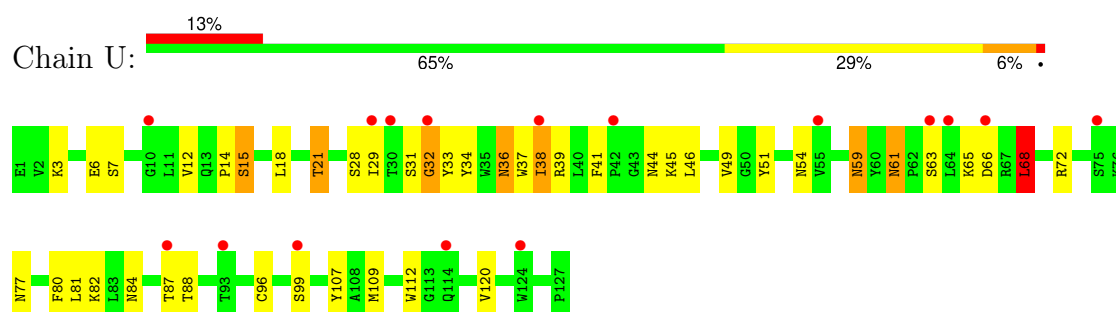
• Molecule 9: Cytochrome b-c1 complex subunit 9



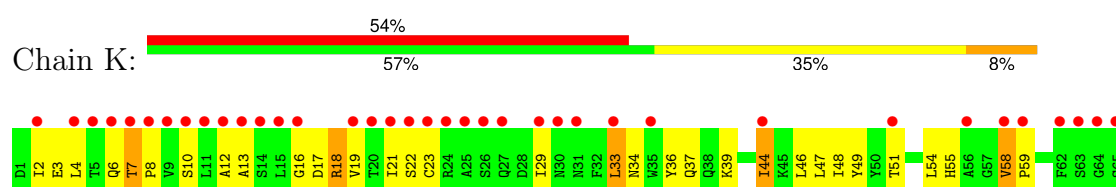
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

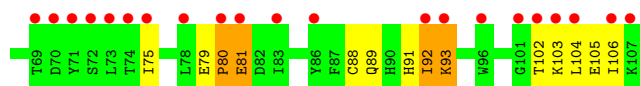


• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

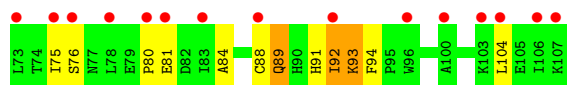
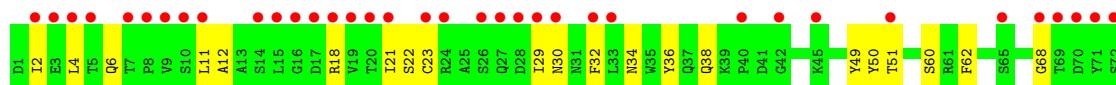


• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

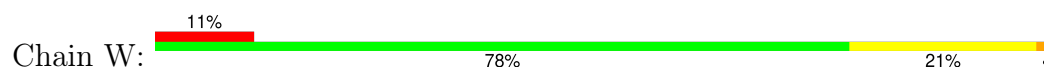




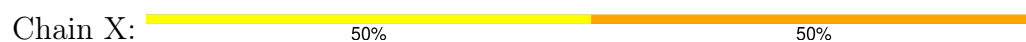
- Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT



- Molecule 12: Cytochrome c iso-2



- 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, α , β , γ	145.54Å 162.97Å 194.23Å 90.00° 104.39° 90.00°	Depositor
Resolution (Å)	19.97 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (19.97-2.50) 95.8 (19.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.66	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.256 0.226 , 0.255	Depositor DCC
R_{free} test set	14494 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	36805	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6PH, 8PE, GLC, CN6, UMQ, 9PE, FRU, FES, M3L, SMA, 7PH, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	0/3405	0.93	12/4614 (0.3%)
1	L	0.44	0/3405	0.96	11/4614 (0.2%)
2	B	0.43	0/2781	0.99	15/3764 (0.4%)
2	M	0.44	0/2781	0.99	14/3764 (0.4%)
3	C	0.52	0/3192	1.00	14/4354 (0.3%)
3	N	0.55	0/3192	1.04	19/4354 (0.4%)
4	D	0.45	0/2001	0.98	4/2726 (0.1%)
4	O	0.46	0/2001	0.99	8/2726 (0.3%)
5	E	0.44	0/1444	0.93	6/1957 (0.3%)
5	P	0.45	0/1444	0.98	7/1957 (0.4%)
6	F	0.38	0/638	0.87	1/858 (0.1%)
6	Q	0.42	0/638	0.94	2/858 (0.2%)
7	G	0.49	1/1032 (0.1%)	0.96	2/1397 (0.1%)
7	R	0.48	0/1032	0.94	1/1397 (0.1%)
8	H	0.46	0/804	0.95	6/1088 (0.6%)
8	S	0.48	0/804	0.96	4/1088 (0.4%)
9	I	0.41	0/461	0.85	1/622 (0.2%)
9	T	0.43	0/461	0.85	0/622
10	J	0.40	0/1043	0.88	2/1422 (0.1%)
10	U	0.38	0/1043	0.89	4/1422 (0.3%)
11	K	0.40	0/863	0.80	2/1172 (0.2%)
11	V	0.39	0/863	0.75	0/1172
12	W	0.40	0/891	0.95	1/1191 (0.1%)
All	All	0.46	1/36219 (0.0%)	0.96	136/49139 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	26	VAL	CA-CB	5.09	1.56	1.54

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	163	GLY	N-CA-C	8.84	125.20	114.69
1	L	356	ILE	N-CA-C	8.43	121.39	112.96
2	B	310	LYS	N-CA-C	-7.88	102.01	112.72
4	D	108	ASP	N-CA-C	7.70	120.65	111.33
6	F	142	LEU	N-CA-C	7.62	120.25	111.11
4	O	108	ASP	N-CA-C	7.62	121.50	111.75
10	J	36	ASN	N-CA-C	7.60	121.71	110.46
2	B	87	ILE	N-CA-C	-7.40	94.38	107.18
3	N	328	ILE	N-CA-C	-7.37	103.34	110.42
2	M	113	ALA	N-CA-C	7.37	119.31	111.28
1	A	239	LYS	N-CA-C	7.36	116.95	108.49
5	E	163	GLY	N-CA-C	7.26	125.34	115.32
3	N	25	SER	N-CA-C	7.20	121.78	112.92
3	C	202	HIS	N-CA-C	7.08	118.99	111.28
2	B	152	ARG	N-CA-C	7.00	125.71	110.80
10	U	36	ASN	N-CA-C	6.97	120.70	110.59
3	C	328	ILE	N-CA-C	-6.97	103.52	110.62
3	C	346	VAL	N-CA-C	6.94	123.88	108.88
6	Q	142	LEU	N-CA-C	6.77	119.23	111.11
2	M	152	ARG	N-CA-C	6.75	121.48	112.30
3	N	384	ASN	N-CA-C	6.75	120.00	111.69
5	P	47	ASN	N-CA-C	-6.74	104.69	113.12
3	N	261	ASN	CA-C-N	6.74	126.43	119.56
3	N	261	ASN	C-N-CA	6.74	126.43	119.56
1	L	382	ASN	N-CA-C	6.67	118.51	109.24
3	N	346	VAL	N-CA-C	6.65	123.24	108.88
6	Q	86	LYS	N-CA-C	-6.62	105.17	113.18
2	B	59	THR	N-CA-C	-6.59	100.45	110.14
7	R	25	CYS	N-CA-C	6.57	119.42	111.40
2	M	123	VAL	N-CA-C	6.54	117.03	110.23
3	C	222	HIS	N-CA-C	6.52	119.75	109.96
2	M	179	VAL	N-CA-C	6.40	118.36	111.58
4	D	83	GLU	N-CA-C	6.37	119.62	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	317	THR	N-CA-C	6.35	119.01	111.33
5	E	180	CYS	N-CA-C	6.34	117.86	111.07
8	S	2	GLY	CA-C-N	6.32	126.89	120.38
8	S	2	GLY	C-N-CA	6.32	126.89	120.38
2	B	84	ARG	N-CA-C	-6.31	105.06	112.89
2	B	155	LEU	N-CA-C	-6.29	105.58	113.20
2	M	87	ILE	N-CA-C	-6.28	96.31	107.18
8	H	53	LYS	N-CA-C	-6.23	105.17	114.64
8	H	60	LEU	N-CA-C	6.18	117.68	111.07
5	P	180	CYS	N-CA-C	6.17	117.80	111.14
3	N	202	HIS	N-CA-C	6.12	117.95	111.28
1	L	286	GLY	N-CA-C	6.01	121.94	111.78
1	A	382	ASN	CA-C-N	5.98	125.53	119.19
1	A	382	ASN	C-N-CA	5.98	125.53	119.19
3	C	185	LEU	N-CA-C	5.96	117.58	111.14
3	N	137	GLY	N-CA-C	-5.94	104.43	112.57
3	C	261	ASN	CA-C-N	5.93	125.63	119.82
3	C	261	ASN	C-N-CA	5.93	125.63	119.82
1	A	200	HIS	N-CA-C	5.89	120.85	113.43
2	M	84	ARG	N-CA-C	-5.87	105.61	112.89
2	M	86	TYR	N-CA-C	5.86	118.39	109.95
2	B	123	VAL	N-CA-C	5.82	115.95	110.30
2	M	334	SER	CA-C-N	5.77	127.06	119.84
2	M	334	SER	C-N-CA	5.77	127.06	119.84
8	H	35	LYS	CA-C-N	5.76	127.04	119.84
8	H	35	LYS	C-N-CA	5.76	127.04	119.84
1	L	46	ALA	N-CA-C	5.74	118.40	111.40
7	G	44	LYS	N-CA-C	-5.72	100.97	110.17
4	O	68	GLY	N-CA-C	-5.71	104.54	112.18
1	A	65	TYR	N-CA-C	5.70	120.29	113.23
5	P	139	ASP	CA-C-N	5.69	126.95	119.84
5	P	139	ASP	C-N-CA	5.69	126.95	119.84
2	B	315	SER	N-CA-C	5.67	122.34	109.81
4	D	73	ALA	N-CA-C	5.64	118.59	107.98
2	B	113	ALA	N-CA-C	5.62	117.40	111.28
10	J	68	LEU	N-CA-C	5.60	118.39	110.50
8	S	50	ARG	N-CA-C	-5.60	104.57	111.40
2	M	111	LYS	N-CA-C	5.57	119.27	111.30
3	N	70	ARG	N-CA-C	5.55	120.06	113.12
1	L	212	GLY	N-CA-C	-5.55	105.44	111.21
3	N	99	LYS	N-CA-C	-5.54	105.24	111.28
5	E	139	ASP	CA-C-N	5.53	126.76	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	139	ASP	C-N-CA	5.53	126.76	119.84
8	H	2	GLY	CA-C-N	5.52	126.06	120.38
8	H	2	GLY	C-N-CA	5.52	126.06	120.38
3	N	264	VAL	N-CA-C	5.51	115.92	107.77
12	W	24	GLN	N-CA-C	5.50	119.61	113.01
4	O	83	GLU	N-CA-C	5.50	118.20	109.24
2	M	59	THR	N-CA-C	-5.49	101.62	110.14
2	B	110	TYR	N-CA-C	5.48	118.43	111.69
3	N	348	TYR	N-CA-C	5.45	117.22	111.28
8	S	60	LEU	N-CA-C	5.44	117.21	111.28
3	C	25	SER	N-CA-C	5.43	119.60	112.92
2	M	169	LEU	N-CA-C	-5.43	105.44	111.36
3	N	215	ASN	N-CA-C	5.43	119.01	112.38
1	A	382	ASN	N-CA-C	5.42	117.44	109.42
4	O	232	ASP	N-CA-C	5.42	119.05	111.74
10	U	33	TYR	N-CA-C	5.41	117.69	109.63
9	I	11	PHE	N-CA-C	5.41	120.55	113.30
3	C	264	VAL	N-CA-C	5.39	115.82	107.78
3	C	107	ARG	N-CA-C	5.39	117.48	110.53
1	L	439	ILE	N-CA-C	5.39	116.70	111.91
2	M	278	LYS	N-CA-C	5.36	117.47	108.73
11	K	58	VAL	CA-C-N	5.32	125.26	119.78
11	K	58	VAL	C-N-CA	5.32	125.26	119.78
2	B	334	SER	CA-C-N	5.30	126.47	119.84
2	B	334	SER	C-N-CA	5.30	126.47	119.84
1	L	380	SER	N-CA-C	-5.30	102.68	110.52
4	D	251	VAL	CB-CA-C	-5.29	105.19	111.97
1	L	382	ASN	CA-C-N	5.28	124.91	119.05
1	L	382	ASN	C-N-CA	5.28	124.91	119.05
4	O	100	VAL	N-CA-C	5.26	116.53	112.12
3	C	273	TRP	N-CA-C	5.25	117.68	111.33
7	G	6	THR	N-CA-C	-5.22	105.48	111.07
10	U	32	GLY	N-CA-C	5.21	125.52	113.18
1	A	356	ILE	N-CA-C	5.19	119.49	113.42
3	C	219	ILE	CA-C-N	5.18	125.12	119.78
3	C	219	ILE	C-N-CA	5.18	125.12	119.78
2	B	191	ASN	N-CA-C	-5.18	106.26	112.58
3	N	219	ILE	CA-C-N	5.16	125.16	119.89
3	N	219	ILE	C-N-CA	5.16	125.16	119.89
5	E	194	GLY	CA-C-N	5.15	125.23	119.87
5	E	194	GLY	C-N-CA	5.15	125.23	119.87
2	M	185	LEU	N-CA-C	5.15	116.89	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	THR	CA-C-N	5.14	124.58	119.24
1	A	172	THR	C-N-CA	5.14	124.58	119.24
1	A	154	ASN	N-CA-C	5.13	120.40	114.04
10	U	68	LEU	N-CA-C	5.12	117.45	110.55
3	N	247	SER	CA-C-N	5.11	124.83	119.82
3	N	247	SER	C-N-CA	5.11	124.83	119.82
5	P	178	CYS	CA-C-N	5.11	124.72	119.56
5	P	178	CYS	C-N-CA	5.11	124.72	119.56
3	N	273	TRP	N-CA-C	5.10	117.23	111.11
1	A	357	SER	N-CA-C	5.09	121.19	112.99
2	B	182	LYS	N-CA-C	5.09	117.22	111.11
1	A	164	LEU	N-CA-C	-5.08	105.82	111.36
2	B	86	TYR	N-CA-C	5.06	117.58	110.14
1	L	66	ASN	N-CA-C	-5.05	106.36	112.88
3	C	137	GLY	N-CA-C	-5.05	104.83	112.41
1	L	379	GLU	N-CA-C	5.03	116.44	109.54
4	O	251	VAL	CB-CA-C	-5.02	105.29	112.22
4	O	155	ILE	CA-C-N	5.01	124.92	119.76
4	O	155	ILE	C-N-CA	5.01	124.92	119.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	279	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3321	101	0
1	L	3344	0	3321	82	0
2	B	2735	0	2774	78	0
2	M	2735	0	2774	78	0
3	C	3090	0	3129	56	0
3	N	3090	0	3129	33	0
4	D	1940	0	1862	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	1940	0	1862	31	0
5	E	1411	0	1386	39	0
5	P	1411	0	1386	26	0
6	F	624	0	581	10	0
6	Q	624	0	581	9	0
7	G	1012	0	1026	22	0
7	R	1012	0	1026	16	0
8	H	773	0	736	15	0
8	S	773	0	736	17	0
9	I	448	0	445	5	0
9	T	448	0	445	7	0
10	J	1015	0	959	30	0
10	U	1015	0	959	38	0
11	K	842	0	820	33	0
11	V	842	0	820	24	0
12	W	885	0	890	15	0
13	X	23	0	21	2	0
14	A	34	0	44	4	0
14	L	34	0	44	2	0
15	C	86	0	60	3	0
15	D	43	0	30	0	0
15	N	86	0	60	1	0
15	O	43	0	30	1	0
15	W	43	0	30	2	0
16	C	37	0	42	1	0
16	N	37	0	42	1	0
17	C	47	0	73	2	0
17	N	47	0	73	2	0
18	C	50	0	56	9	0
18	N	50	0	56	5	0
19	C	40	0	59	0	0
19	N	40	0	59	0	0
20	D	38	0	55	3	0
20	O	38	0	55	2	0
21	E	4	0	0	0	0
21	P	4	0	0	1	0
22	E	40	0	59	2	0
22	L	40	0	59	0	0
23	A	42	0	0	0	0
23	B	17	0	0	1	0
23	C	75	0	0	4	0
23	D	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	E	19	0	0	0	0
23	F	3	0	0	0	0
23	G	21	0	0	1	0
23	H	10	0	0	0	0
23	I	4	0	0	0	0
23	J	2	0	0	1	0
23	K	1	0	0	0	0
23	L	54	0	0	2	0
23	M	15	0	0	0	0
23	N	88	0	0	3	0
23	O	74	0	0	2	0
23	P	18	0	0	0	0
23	Q	3	0	0	0	0
23	R	22	0	0	1	0
23	S	13	0	0	0	0
23	T	5	0	0	0	0
23	U	2	0	0	0	0
23	W	10	0	0	1	0
All	All	36805	0	35975	749	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (749) 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:M:347:LYS:HD3	2:M:347:LYS:H	1.19	1.01
1:A:63:ASN:H	1:A:66:ASN:HD21	1.06	1.00
1:A:382:ASN:HD21	1:A:384:VAL:HG22	1.22	0.99
1:L:63:ASN:H	1:L:66:ASN:ND2	1.60	0.99
6:Q:77:GLN:H	6:Q:77:GLN:HE21	1.08	0.98
6:F:77:GLN:H	6:F:77:GLN:HE21	0.96	0.93
11:V:75:ILE:HG22	11:V:76:SER:H	1.35	0.90
1:L:63:ASN:H	1:L:66:ASN:HD21	0.94	0.90
6:F:77:GLN:H	6:F:77:GLN:NE2	1.69	0.90
6:F:78:LEU:HD13	6:F:142:LEU:HD22	1.52	0.89
6:Q:77:GLN:H	6:Q:77:GLN:NE2	1.73	0.86
1:A:58:GLY:H	1:A:61:ASN:HD22	1.24	0.86
2:M:49:HIS:HD2	2:M:161:TYR:H	1.24	0.85
1:L:317:HIS:HE1	1:L:351:TRP:HE1	1.23	0.84
2:M:62:ARG:HG2	2:M:62:ARG:HH21	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:29:ILE:H	10:U:77:ASN:HD21	1.25	0.84
5:E:134:MET:HG3	10:J:31:SER:HB3	1.61	0.81
11:V:93:LYS:HZ3	11:V:94:PHE:H	1.29	0.81
2:M:150:THR:HG22	2:M:352:ASN:HD22	1.45	0.81
11:K:21:ILE:HG22	11:K:22:SER:H	1.47	0.78
2:B:181:THR:HB	2:B:212:GLY:H	1.47	0.78
6:F:77:GLN:HE21	6:F:77:GLN:N	1.78	0.78
10:J:29:ILE:HG12	10:J:77:ASN:ND2	1.99	0.77
2:M:246:ASN:HD22	2:M:246:ASN:H	1.32	0.77
1:A:429:GLN:HA	1:A:429:GLN:HE21	1.48	0.76
1:L:179:ARG:HG2	1:L:179:ARG:HH21	1.49	0.76
10:J:99:SER:HB3	10:J:109:MET:HG2	1.69	0.75
2:M:347:LYS:HD3	2:M:347:LYS:N	1.98	0.75
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.67	0.75
2:B:49:HIS:HD2	2:B:161:TYR:H	1.34	0.75
1:L:344:ILE:HG21	1:L:448:ILE:HD12	1.68	0.75
2:B:62:ARG:HG2	2:B:62:ARG:HH21	1.50	0.75
5:E:44:LYS:NZ	5:E:52:GLY:H	1.83	0.75
2:M:49:HIS:CD2	2:M:161:TYR:H	2.05	0.75
9:T:8:LYS:O	9:T:12:LYS:HG3	1.87	0.75
11:V:6:GLN:HG2	11:V:23:CYS:SG	2.27	0.74
2:M:150:THR:HG22	2:M:352:ASN:ND2	2.03	0.74
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.23	0.74
7:R:77:ARG:HD3	7:R:88:LEU:HD11	1.69	0.74
1:L:63:ASN:N	1:L:66:ASN:HD21	1.79	0.74
2:M:238:VAL:HG13	2:M:356:VAL:HB	1.68	0.74
4:O:96:VAL:HB	4:O:251:VAL:HG13	1.69	0.73
1:A:73:TRP:CE3	1:A:76:ILE:HD11	2.24	0.73
1:L:58:GLY:H	1:L:61:ASN:HD22	1.37	0.73
3:N:208:ASN:HD22	3:N:210:LEU:H	1.36	0.73
2:B:336:ILE:HD12	2:B:336:ILE:H	1.54	0.73
2:B:238:VAL:HG13	2:B:356:VAL:HB	1.71	0.72
1:A:382:ASN:ND2	1:A:384:VAL:HG22	2.01	0.72
2:B:300:ASN:O	2:B:304:ILE:HG12	1.89	0.72
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.38	0.72
3:C:208:ASN:HD22	3:C:210:LEU:H	1.38	0.72
1:A:63:ASN:H	1:A:66:ASN:ND2	1.83	0.71
5:E:172:ASP:H	5:E:184:HIS:HD2	1.38	0.71
17:N:4110:8PE:H1A	8:S:51:ARG:HE	1.56	0.71
4:D:272:LYS:O	4:D:276:ILE:HG22	1.90	0.71
2:M:137:CYS:SG	2:M:139:VAL:HG22	2.31	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:324:LYS:O	2:M:327:VAL:HG22	1.90	0.71
1:L:317:HIS:CE1	1:L:351:TRP:HE1	2.06	0.70
2:M:347:LYS:HG2	2:M:348:LEU:H	1.55	0.70
1:A:228:LEU:HG	1:A:229:SER:H	1.56	0.70
18:C:4031:CN6:HAA	7:G:85:HIS:NE2	2.06	0.70
1:L:241:LYS:H	1:L:241:LYS:HD2	1.57	0.69
3:N:214:GLY:O	3:N:218:ARG:HD2	1.93	0.69
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.73	0.69
2:B:30:THR:HG23	2:B:190:GLU:HB3	1.74	0.69
3:C:214:GLY:O	3:C:218:ARG:HD2	1.92	0.69
1:A:66:ASN:HD22	1:A:66:ASN:H	1.41	0.69
11:K:29:ILE:HG22	11:K:92:ILE:HD12	1.74	0.69
11:K:47:LEU:HA	11:K:58:VAL:HG11	1.74	0.69
18:N:4131:CN6:HAA	7:R:85:HIS:NE2	2.08	0.68
18:N:4131:CN6:HC	23:N:6998:HOH:O	1.92	0.68
3:C:107:ARG:HH21	3:C:107:ARG:HG3	1.58	0.68
1:A:361:THR:HG21	7:R:123:ILE:O	1.94	0.68
10:J:114:GLN:H	10:J:114:GLN:NE2	1.92	0.68
5:P:44:LYS:NZ	5:P:52:GLY:H	1.91	0.68
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.59	0.67
1:A:127:GLN:HG2	1:A:130:ASN:HD22	1.60	0.67
1:A:217:GLU:HA	1:A:220:VAL:HG12	1.76	0.67
3:N:323:LYS:CE	8:S:55:GLN:HE22	2.08	0.67
1:L:130:ASN:N	1:L:130:ASN:HD22	1.92	0.66
10:J:61:ASN:HD22	10:J:63:SER:H	1.44	0.66
8:H:56:PHE:O	8:H:60:LEU:HB2	1.96	0.66
5:P:172:ASP:H	5:P:184:HIS:HD2	1.43	0.66
10:J:38:ILE:HD11	10:J:46:LEU:HD22	1.78	0.66
10:U:61:ASN:HD22	10:U:63:SER:H	1.42	0.66
2:M:300:ASN:O	2:M:304:ILE:HG12	1.96	0.65
23:O:6502:HOH:O	12:W:25:GLN:HG3	1.95	0.65
3:C:185:LEU:HG	3:N:48:ILE:HD13	1.79	0.65
5:P:132:VAL:HG21	5:P:192:ARG:NH1	2.11	0.65
1:A:66:ASN:HA	1:A:188:LEU:HD11	1.79	0.65
10:U:41:PHE:HB2	10:U:45:LYS:HG3	1.79	0.65
1:L:172:THR:HG23	1:L:242:ALA:HA	1.79	0.64
4:D:147:ARG:HH21	4:D:150:LYS:HE3	1.62	0.64
3:C:253:HIS:HD2	3:C:255:ASP:H	1.45	0.64
9:T:52:VAL:HA	9:T:55:ARG:HD3	1.77	0.64
2:B:152:ARG:HH12	2:M:366:ASP:HB2	1.62	0.63
1:L:156:HIS:HD2	1:L:159:ARG:HH21	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:228:LEU:HG	1:L:229:SER:H	1.63	0.63
1:L:270:VAL:O	1:L:271:ASN:HB2	1.97	0.63
6:Q:77:GLN:HE21	6:Q:77:GLN:N	1.88	0.63
4:O:227:ARG:HH11	4:O:244:THR:HG21	1.63	0.63
2:M:31:LEU:HD12	2:M:105:LEU:HD12	1.81	0.63
5:P:103:LEU:O	5:P:120:HIS:HB3	1.98	0.63
5:E:106:ASN:ND2	5:E:119:ARG:HB2	2.14	0.62
1:A:57:SER:O	1:A:102:GLN:HG3	1.99	0.62
3:N:323:LYS:NZ	8:S:55:GLN:HE22	1.98	0.62
1:A:99:ARG:HD3	1:A:174:LEU:HD12	1.80	0.62
3:C:27:ASN:HB2	18:C:4031:CN6:O2'	1.99	0.62
2:M:329:ASN:N	2:M:329:ASN:HD22	1.98	0.62
5:E:58:PHE:HD2	5:E:59:MET:HE2	1.65	0.62
1:A:276:PHE:HZ	1:A:401:LEU:HD21	1.64	0.62
7:G:62:ARG:HD2	2:M:121:GLU:OE2	1.98	0.62
3:N:218:ARG:HG3	8:S:16:MET:HE3	1.81	0.62
1:A:172:THR:HG23	1:A:242:ALA:HA	1.82	0.62
1:L:179:ARG:HG2	1:L:179:ARG:NH2	2.14	0.62
2:M:336:ILE:H	2:M:336:ILE:HD12	1.65	0.62
2:B:152:ARG:O	2:B:153:LYS:HB2	2.00	0.62
2:M:315:SER:N	2:M:316:PRO:HD3	2.15	0.62
10:U:38:ILE:HD11	10:U:46:LEU:HD22	1.80	0.62
2:M:83:ASP:HB2	2:M:86:TYR:H	1.65	0.61
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.83	0.61
3:N:253:HIS:HD2	3:N:255:ASP:H	1.48	0.61
7:R:77:ARG:HD2	23:R:5803:HOH:O	1.99	0.61
5:E:172:ASP:H	5:E:184:HIS:CD2	2.18	0.61
11:K:21:ILE:HG22	11:K:22:SER:N	2.15	0.61
1:L:72:LEU:HD23	1:L:193:LEU:HD21	1.81	0.61
7:G:77:ARG:HD2	23:G:5303:HOH:O	2.00	0.61
4:O:213:ASN:OD1	13:X:2:FRU:H62	2.00	0.61
10:U:68:LEU:HA	10:U:82:LYS:O	2.01	0.61
1:L:207:VAL:HG11	1:L:394:VAL:HG21	1.81	0.61
6:Q:78:LEU:HD13	6:Q:142:LEU:HD22	1.83	0.61
10:U:14:PRO:O	10:U:15:SER:HB3	2.01	0.61
3:C:44:ILE:O	3:C:48:ILE:HG12	2.01	0.60
1:L:149:GLN:O	1:L:153:ASP:HB2	2.02	0.60
2:B:152:ARG:HD3	2:B:224:PHE:CE1	2.36	0.60
7:G:43:LEU:HD21	7:G:78:ALA:CB	2.32	0.60
11:V:2:ILE:HD12	11:V:2:ILE:H	1.66	0.60
10:J:30:THR:O	10:J:54:ASN:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4021:UMQ:HK1	22:E:4013:6PH:H39	1.83	0.60
3:N:253:HIS:CD2	3:N:255:ASP:H	2.19	0.60
11:V:34:ASN:ND2	11:V:50:TYR:H	1.99	0.60
2:M:65:LEU:O	2:M:69:ARG:HG2	2.00	0.60
3:C:4:ARG:HE	3:C:14:ASN:HD21	1.50	0.60
3:C:4:ARG:HE	3:C:14:ASN:ND2	1.99	0.60
1:L:229:SER:HB3	1:L:232:THR:HG21	1.84	0.60
11:K:2:ILE:HD12	11:K:2:ILE:H	1.67	0.59
10:U:41:PHE:HB2	10:U:45:LYS:CG	2.32	0.59
5:P:58:PHE:HD2	5:P:59:MET:HE2	1.67	0.59
1:A:169:PHE:O	1:A:172:THR:HB	2.01	0.59
2:M:68:VAL:O	2:M:72:GLU:HG3	2.01	0.59
4:O:109:ARG:HG3	4:O:178:SER:CB	2.32	0.59
8:H:12:TRP:CE2	8:S:3:PRO:HG3	2.38	0.59
3:N:27:ASN:HB2	18:N:4131:CN6:O2'	2.02	0.59
4:O:78:HIS:HD2	23:O:5586:HOH:O	1.85	0.59
10:U:29:ILE:H	10:U:77:ASN:ND2	1.98	0.59
1:A:38:VAL:HA	1:A:208:VAL:HG13	1.85	0.59
5:E:93:LYS:HG3	5:E:214:VAL:O	2.02	0.59
2:M:246:ASN:H	2:M:246:ASN:ND2	1.99	0.59
10:U:28:SER:HB3	10:U:31:SER:OG	2.02	0.59
7:G:26:VAL:HG12	7:G:30:ASN:HD21	1.68	0.59
12:W:58:THR:HG22	12:W:61:ASN:H	1.68	0.59
1:L:394:VAL:HG12	1:L:399:SER:HA	1.85	0.59
1:A:117:LEU:HD11	1:A:219:LEU:HD12	1.84	0.58
4:D:247:MET:O	4:D:251:VAL:HG22	2.03	0.58
1:A:127:GLN:HG2	1:A:130:ASN:ND2	2.18	0.58
1:A:172:THR:HG23	1:A:173:PRO:HD2	1.85	0.58
4:O:201:GLU:HG3	4:O:202:PRO:HD2	1.86	0.58
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.84	0.58
1:L:382:ASN:OD1	1:L:384:VAL:HG22	2.03	0.58
2:M:308:LEU:HB2	2:M:348:LEU:HD22	1.85	0.58
1:A:289:ASN:C	1:A:289:ASN:HD22	2.11	0.58
11:K:34:ASN:HD22	11:K:49:TYR:HA	1.67	0.58
11:V:2:ILE:HD12	11:V:2:ILE:N	2.19	0.58
11:V:75:ILE:HG22	11:V:76:SER:N	2.14	0.58
3:N:147:ILE:O	3:N:150:LEU:HB2	2.03	0.58
3:N:208:ASN:HB2	3:N:209:PRO:HD2	1.86	0.58
5:P:51:LYS:HE2	5:P:55:TYR:CE1	2.39	0.58
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.04	0.58
3:C:40:LEU:HD12	15:C:4001:HEM:HBB1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:4121:UMQ:O2'	9:T:18:VAL:HG22	2.04	0.58
2:B:49:HIS:CD2	2:B:161:TYR:H	2.19	0.57
2:M:146:LEU:O	2:M:150:THR:HG23	2.03	0.57
2:M:313:ASP:HB3	2:M:344:LYS:O	2.04	0.57
8:S:61:ILE:HB	8:S:62:PRO:HD3	1.85	0.57
1:A:234:THR:HG22	1:A:235:LYS:H	1.70	0.57
10:U:107:TYR:H	11:V:91:HIS:CD2	2.22	0.57
1:A:160:VAL:CG2	1:A:436:THR:HG22	2.35	0.57
3:C:173:ASN:HB3	3:C:174:PRO:HD3	1.85	0.57
8:H:12:TRP:CZ2	8:S:3:PRO:HG3	2.40	0.57
7:R:19:PRO:O	7:R:23:LYS:HG3	2.05	0.56
10:J:24:VAL:HG21	10:J:29:ILE:HD11	1.85	0.56
1:L:172:THR:CG2	1:L:242:ALA:HA	2.35	0.56
5:E:103:LEU:O	5:E:120:HIS:HB3	2.05	0.56
11:V:36:TYR:HE2	11:V:89:GLN:HG2	1.69	0.56
5:P:172:ASP:H	5:P:184:HIS:CD2	2.23	0.56
6:F:81:LEU:HB3	6:F:138:THR:HG22	1.88	0.56
8:H:80:LEU:HB3	8:H:89:LEU:HD23	1.87	0.56
2:B:366:ASP:CB	2:M:152:ARG:HH12	2.19	0.56
10:U:59:ASN:HD22	10:U:59:ASN:C	2.13	0.56
2:B:155:LEU:H	2:B:155:LEU:HD12	1.71	0.55
11:K:4:LEU:HD23	11:K:23:CYS:HB3	1.87	0.55
5:E:106:ASN:HD22	5:E:119:ARG:HB2	1.71	0.55
9:I:8:LYS:O	9:I:12:LYS:HD2	2.06	0.55
2:M:347:LYS:HG2	2:M:348:LEU:N	2.20	0.55
1:A:202:LEU:HD13	1:A:234:THR:HB	1.88	0.55
2:B:197:LEU:O	2:B:201:VAL:HG23	2.06	0.55
3:C:147:ILE:O	3:C:150:LEU:HB2	2.06	0.55
10:U:54:ASN:H	10:U:54:ASN:HD22	1.53	0.55
11:V:93:LYS:NZ	11:V:94:PHE:H	2.01	0.55
2:B:238:VAL:CG1	2:B:356:VAL:HB	2.36	0.55
10:J:61:ASN:ND2	10:J:63:SER:H	2.04	0.55
5:E:103:LEU:HG	5:E:122:THR:HG22	1.89	0.55
3:C:193:MET:HA	3:C:193:MET:HE2	1.87	0.55
1:L:74:LYS:HG3	1:L:95:SER:HB3	1.89	0.55
5:P:55:TYR:O	5:P:59:MET:HG2	2.07	0.55
12:W:96:LYS:HD3	12:W:98:LYS:NZ	2.22	0.55
14:A:4021:UMQ:O2'	9:I:18:VAL:HG22	2.07	0.55
3:C:253:HIS:CD2	3:C:255:ASP:H	2.24	0.55
8:H:83:LYS:O	8:H:86:ARG:HG2	2.06	0.55
5:P:38:ASN:HD21	5:P:40:ASP:CG	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ALA:O	1:A:47:HIS:HB2	2.07	0.54
11:K:6:GLN:HG2	11:K:23:CYS:SG	2.47	0.54
5:P:118:ILE:HG12	5:P:154:ILE:HG12	1.89	0.54
12:W:50:GLY:HA2	12:W:57:TYR:CE1	2.42	0.54
3:C:304:VAL:HG12	3:C:308:THR:HG23	1.89	0.54
20:D:4014:7PH:H35	5:E:70:GLY:HA3	1.88	0.54
11:V:11:LEU:HG	11:V:12:ALA:H	1.72	0.54
1:L:29:VAL:HG12	1:L:30:THR:N	2.22	0.54
1:L:313:ASP:OD1	1:L:335:ARG:HD3	2.07	0.54
2:B:152:ARG:HG2	2:M:364:TYR:CE1	2.43	0.54
3:C:193:MET:HE1	3:C:196:MET:SD	2.48	0.54
5:E:63:MET:HE3	22:E:4013:6PH:H35	1.89	0.54
10:J:40:LEU:O	10:J:92:ALA:HB1	2.07	0.54
1:L:156:HIS:HD2	1:L:159:ARG:NH2	2.04	0.54
4:O:227:ARG:NH1	4:O:244:THR:HG21	2.22	0.54
11:V:38:GLN:O	11:V:84:ALA:HB1	2.07	0.54
2:B:151:PHE:O	2:B:153:LYS:N	2.37	0.54
2:M:152:ARG:HD3	2:M:224:PHE:CE1	2.43	0.54
7:G:43:LEU:HD21	7:G:78:ALA:HB2	1.90	0.54
1:L:241:LYS:H	1:L:241:LYS:CD	2.15	0.54
4:D:109:ARG:HG3	4:D:178:SER:CB	2.38	0.54
4:D:276:ILE:HD13	20:D:4014:7PH:O32	2.07	0.54
1:L:227:ASN:HD22	1:L:228:LEU:H	1.56	0.53
4:O:286:TRP:CE3	5:P:59:MET:HG3	2.43	0.53
1:A:207:VAL:HG11	1:A:394:VAL:HG21	1.90	0.53
2:M:137:CYS:HG	2:M:139:VAL:HG22	1.73	0.53
10:J:61:ASN:HD22	10:J:62:PRO:N	2.05	0.53
1:L:258:LYS:HG2	1:L:335:ARG:HG3	1.91	0.53
2:M:115:LYS:HB2	2:M:118:GLU:HG3	1.89	0.53
3:C:14:ASN:ND2	3:C:18:ILE:HB	2.24	0.53
4:O:125:VAL:HA	4:O:128:MET:HE3	1.89	0.53
11:V:21:ILE:HG22	11:V:22:SER:N	2.24	0.53
2:M:197:LEU:O	2:M:201:VAL:HG23	2.09	0.53
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.22	0.53
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.24	0.53
18:N:4131:CN6:HAA	7:R:85:HIS:CE1	2.43	0.53
4:O:247:MET:O	4:O:251:VAL:HG22	2.09	0.53
2:B:65:LEU:O	2:B:69:ARG:HG2	2.09	0.53
3:C:15:SER:O	3:C:202:HIS:HE1	1.92	0.53
4:O:72:PRO:HB2	6:Q:139:ALA:HB2	1.90	0.53
10:U:18:LEU:O	10:U:82:LYS:HA	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLN:HG3	1:A:374:LEU:N	2.24	0.52
1:L:46:ALA:O	1:L:47:HIS:HB2	2.08	0.52
1:A:86:ALA:HB2	1:A:119:PHE:CZ	2.44	0.52
2:B:49:HIS:HE1	2:B:130:ASP:OD1	1.93	0.52
2:B:83:ASP:HB2	2:B:86:TYR:H	1.74	0.52
3:N:301:VAL:O	3:N:304:VAL:HG12	2.09	0.52
10:U:38:ILE:HD13	10:U:112:TRP:HH2	1.73	0.52
5:E:134:MET:HG3	10:J:31:SER:CB	2.35	0.52
6:F:91:GLY:O	6:F:95:VAL:HG13	2.10	0.52
3:N:4:ARG:HE	3:N:14:ASN:ND2	2.07	0.52
5:P:115:PRO:HD2	5:P:158:ILE:HD11	1.91	0.52
1:L:252:ARG:HD3	1:L:254:ASP:OD1	2.10	0.52
2:M:260:LEU:O	2:M:271:ILE:HD11	2.10	0.52
1:A:179:ARG:HH21	1:A:179:ARG:HG2	1.74	0.52
1:A:181:THR:O	1:A:185:LEU:HB2	2.10	0.52
2:B:35:VAL:CG1	2:B:179:VAL:HG12	2.40	0.52
15:C:4002:HEM:HMB1	15:C:4002:HEM:HBB2	1.92	0.52
4:D:69:LEU:HD23	6:F:128:PHE:CD1	2.45	0.52
5:E:65:LEU:HD21	9:I:24:GLY:C	2.35	0.52
1:L:241:LYS:HD2	1:L:241:LYS:N	2.24	0.52
3:C:25:SER:OG	7:G:79:HIS:HD2	1.93	0.51
3:C:184:TYR:CD1	15:C:4001:HEM:HBC1	2.45	0.51
3:N:4:ARG:HE	3:N:14:ASN:HD21	1.56	0.51
3:N:335:LEU:O	3:N:339:ILE:HG12	2.10	0.51
1:L:182:LEU:O	1:L:186:GLU:HG2	2.10	0.51
1:A:306:ILE:HA	1:A:311:LEU:HD22	1.92	0.51
4:O:92:ARG:HG2	4:O:236:TYR:CD2	2.46	0.51
4:O:231:ASP:OD1	4:O:244:THR:HG23	2.09	0.51
20:O:4114:7PH:H25	20:O:4114:7PH:H29	1.93	0.51
10:U:49:VAL:CG1	10:U:68:LEU:HD23	2.41	0.51
11:V:29:ILE:HG22	11:V:92:ILE:HD12	1.93	0.51
12:W:36:LYS:HB3	23:W:7422:HOH:O	2.10	0.51
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.92	0.51
2:B:264:LEU:HD12	2:B:317:ALA:HB2	1.92	0.51
18:C:4031:CN6:HC	23:C:6590:HOH:O	2.11	0.51
2:B:232:ARG:NH1	2:M:164:VAL:HG21	2.26	0.51
3:C:58:ILE:H	3:C:173:ASN:HD22	1.58	0.51
6:F:117:LEU:C	6:F:119:HIS:H	2.19	0.51
2:M:62:ARG:HH21	2:M:62:ARG:CG	2.17	0.51
2:M:315:SER:HB3	2:M:344:LYS:HA	1.93	0.51
12:W:28:THR:HG23	12:W:36:LYS:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:247:LYS:O	2:M:250:LEU:HD22	2.10	0.51
2:B:183:GLU:HB2	2:B:213:LYS:O	2.10	0.51
10:J:107:TYR:H	11:K:91:HIS:CD2	2.29	0.51
11:K:17:ASP:HB2	11:K:18:ARG:HH21	1.75	0.51
2:M:298:SER:O	2:M:302:LYS:HB2	2.11	0.51
2:B:62:ARG:HH21	2:B:62:ARG:CG	2.24	0.50
3:C:218:ARG:HG3	8:H:16:MET:HE3	1.93	0.50
4:D:92:ARG:HG2	4:D:236:TYR:CD2	2.45	0.50
4:O:135:ASP:OD2	4:O:146:LYS:HE2	2.11	0.50
1:A:350:GLN:O	1:A:353:ARG:HB2	2.12	0.50
2:B:255:VAL:HG12	2:B:321:THR:HG21	1.94	0.50
2:B:364:TYR:CZ	2:M:152:ARG:HG2	2.46	0.50
2:M:26:THR:HG21	2:M:191:ASN:HD21	1.77	0.50
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.76	0.50
2:B:246:ASN:HB2	2:B:249:SER:HB3	1.93	0.50
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.92	0.50
3:N:320:VAL:HG13	8:S:58:TYR:HE2	1.76	0.50
10:U:38:ILE:HD13	10:U:112:TRP:CH2	2.46	0.50
10:U:87:THR:O	10:U:120:VAL:HG21	2.10	0.50
11:V:21:ILE:HG22	11:V:22:SER:H	1.75	0.50
1:L:179:ARG:H	1:L:179:ARG:HD2	1.76	0.50
2:M:308:LEU:CB	2:M:348:LEU:HD22	2.41	0.50
1:A:239:LYS:HD2	1:A:239:LYS:N	2.25	0.50
1:A:345:HIS:O	1:A:349:LYS:HB2	2.12	0.50
5:P:44:LYS:HB3	8:S:35:LYS:HG3	1.92	0.50
1:A:99:ARG:HD3	1:A:174:LEU:CD1	2.41	0.50
1:A:164:LEU:HD13	1:A:327:LEU:HD13	1.94	0.50
1:A:214:ILE:O	1:A:214:ILE:HD12	2.11	0.50
3:C:107:ARG:HG3	3:C:107:ARG:NH2	2.27	0.50
11:K:37:GLN:HB2	11:K:47:LEU:HD11	1.91	0.50
1:L:63:ASN:N	1:L:66:ASN:ND2	2.44	0.50
7:R:97:GLN:H	7:R:97:GLN:NE2	2.10	0.50
1:A:198:ASN:O	1:A:202:LEU:HD21	2.11	0.50
4:O:286:TRP:CD2	5:P:59:MET:HG3	2.46	0.50
2:B:326:ALA:C	2:B:328:GLN:H	2.20	0.50
1:A:172:THR:HG21	1:A:243:ALA:H	1.77	0.50
3:C:313:VAL:HG22	3:C:319:LYS:HE3	1.94	0.50
8:H:35:LYS:O	8:H:37:LEU:N	2.34	0.50
3:C:229:ASP:O	3:C:233:VAL:HG23	2.12	0.49
3:C:313:VAL:HG22	3:C:319:LYS:CE	2.43	0.49
1:L:238:LEU:N	1:L:238:LEU:HD22	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:313:ASP:C	2:M:315:SER:H	2.20	0.49
1:A:350:GLN:HE22	1:A:353:ARG:HH21	1.59	0.49
1:A:397:LYS:HG3	1:A:399:SER:O	2.13	0.49
1:L:375:GLY:HA3	2:M:28:ILE:HG13	1.93	0.49
4:O:163:GLN:H	4:O:163:GLN:NE2	2.11	0.49
4:O:301:VAL:CG2	8:S:25:THR:HB	2.42	0.49
3:C:222:HIS:O	3:C:223:SER:HB2	2.13	0.49
3:C:14:ASN:HD22	3:C:18:ILE:HB	1.76	0.49
3:C:326:PHE:CZ	17:C:4010:8PE:H34A	2.47	0.49
3:C:77:ILE:O	3:C:81:LEU:HB2	2.13	0.49
3:C:110:ARG:NH2	3:C:205:GLY:O	2.46	0.49
1:L:29:VAL:HG12	1:L:30:THR:H	1.75	0.49
1:A:265:VAL:HG21	1:A:426:LEU:HD13	1.94	0.49
1:A:275:TYR:CZ	1:A:279:LYS:HE2	2.46	0.49
11:K:103:LYS:HG2	11:K:104:LEU:H	1.78	0.49
1:L:57:SER:HA	1:L:61:ASN:ND2	2.28	0.49
2:M:310:LYS:HE3	2:M:312:LYS:HB3	1.94	0.49
3:C:104:GLY:HA2	3:C:106:TYR:CE2	2.48	0.49
3:C:326:PHE:HZ	17:C:4010:8PE:H34A	1.78	0.49
10:U:7:SER:OG	10:U:21:THR:HG23	2.12	0.49
11:V:11:LEU:HG	11:V:12:ALA:N	2.27	0.49
1:A:235:LYS:HB2	1:A:235:LYS:NZ	2.26	0.49
11:K:12:ALA:HA	11:K:105:GLU:O	2.13	0.49
1:L:306:ILE:HA	1:L:311:LEU:HD22	1.94	0.49
3:N:76:TYR:CG	4:O:262:GLU:HG3	2.48	0.49
1:A:302:LEU:HB2	1:A:350:GLN:HG3	1.95	0.49
7:G:91:ASN:H	7:G:91:ASN:ND2	2.10	0.49
1:L:172:THR:HG23	1:L:173:PRO:HD2	1.95	0.49
2:M:62:ARG:NH2	2:M:67:LEU:HD13	2.28	0.49
3:N:320:VAL:HG23	23:N:6971:HOH:O	2.13	0.49
5:P:168:GLY:HA2	5:P:176:TRP:CD1	2.47	0.49
12:W:26:CYS:HB3	12:W:37:VAL:HB	1.94	0.49
1:A:122:GLN:HG3	1:A:126:GLN:NE2	2.28	0.48
2:M:44:LYS:O	2:M:47:VAL:HG23	2.13	0.48
1:A:247:SER:O	1:A:432:ALA:HA	2.13	0.48
18:C:4031:CN6:O14	4:D:288:LYS:NZ	2.46	0.48
5:E:93:LYS:HE3	5:E:213:ILE:HD11	1.94	0.48
12:W:20:LYS:HA	12:W:24:GLN:HG2	1.94	0.48
1:A:280:LEU:HD13	1:A:413:ILE:HG21	1.96	0.48
10:J:87:THR:HG22	10:J:88:THR:N	2.28	0.48
1:L:230:LEU:HD13	1:L:231:GLN:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:THR:HB	1:A:216:HIS:CD2	2.48	0.48
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.61	0.48
2:B:193:VAL:HG23	2:B:193:VAL:O	2.12	0.48
5:E:122:THR:O	5:E:126:ILE:HG13	2.13	0.48
2:M:347:LYS:O	2:M:348:LEU:HB2	2.12	0.48
1:A:172:THR:CG2	1:A:242:ALA:HA	2.43	0.48
2:B:52:ASN:ND2	2:B:80:SER:OG	2.45	0.48
1:L:73:TRP:CE3	1:L:76:ILE:HD11	2.47	0.48
1:L:429:GLN:HA	1:L:429:GLN:OE1	2.14	0.48
1:A:86:ALA:HB2	1:A:119:PHE:CE1	2.48	0.48
3:C:220:PRO:HB2	23:C:7439:HOH:O	2.13	0.48
3:C:234:PHE:CZ	4:D:280:LEU:HG	2.49	0.48
10:J:51:TYR:C	10:J:51:TYR:CD2	2.91	0.48
1:L:172:THR:HG21	1:L:243:ALA:H	1.78	0.48
1:A:36:ILE:HA	1:A:203:ASN:HD21	1.79	0.48
1:A:58:GLY:H	1:A:61:ASN:ND2	2.02	0.48
5:E:146:ARG:CZ	5:E:202:ILE:HD11	2.44	0.48
4:O:136:ASP:HB3	4:O:145:LYS:HG3	1.96	0.48
7:R:53:ASN:ND2	7:R:56:MET:H	2.11	0.48
1:A:121:ASN:O	1:A:125:ILE:HB	2.14	0.48
2:B:35:VAL:HG12	2:B:179:VAL:HG12	1.96	0.48
2:B:104:ALA:O	2:B:108:VAL:HG23	2.14	0.48
2:M:305:VAL:O	2:M:309:LYS:HG2	2.14	0.48
11:V:50:TYR:O	11:V:51:THR:HG22	2.13	0.48
8:H:48:SER:C	8:H:50:ARG:H	2.21	0.48
1:L:141:LYS:HE3	1:L:186:GLU:HA	1.94	0.48
6:Q:91:GLY:O	6:Q:95:VAL:HG13	2.14	0.48
2:B:315:SER:N	2:B:316:PRO:HD3	2.29	0.47
4:D:286:TRP:HZ3	5:E:56:ALA:HA	1.79	0.47
17:N:4110:8PE:H37A	17:N:4110:8PE:H3AA	1.66	0.47
4:O:109:ARG:HG3	4:O:178:SER:HB2	1.96	0.47
6:Q:90:GLU:HG2	6:Q:133:TYR:CE1	2.50	0.47
10:U:51:TYR:C	10:U:51:TYR:CD2	2.91	0.47
5:E:187:ILE:HG13	5:E:187:ILE:O	2.14	0.47
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.44	0.47
11:K:2:ILE:HD12	11:K:2:ILE:N	2.30	0.47
2:M:318:ILE:O	2:M:321:THR:HG22	2.14	0.47
3:N:222:HIS:O	3:N:223:SER:HB2	2.14	0.47
1:L:28:GLU:O	1:L:41:GLU:HG3	2.13	0.47
1:L:76:ILE:HG23	1:L:140:THR:HG21	1.95	0.47
5:P:43:LEU:HD21	8:S:29:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:18:LEU:O	10:J:82:LYS:HA	2.14	0.47
1:A:141:LYS:O	1:A:145:LEU:HB2	2.15	0.47
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.96	0.47
4:D:227:ARG:HH11	4:D:244:THR:HG21	1.80	0.47
5:E:154:ILE:HD12	5:E:205:TYR:CE2	2.50	0.47
1:L:67:ASN:ND2	1:L:180:GLY:HA2	2.29	0.47
14:A:4021:UMQ:HC1	9:I:18:VAL:CG1	2.45	0.47
5:E:51:LYS:HD2	8:H:36:PRO:HG3	1.96	0.47
1:L:66:ASN:H	1:L:66:ASN:HD22	1.63	0.47
1:L:67:ASN:HD21	1:L:177:PRO:HG2	1.80	0.47
1:L:169:PHE:HB3	1:L:172:THR:HG22	1.96	0.47
15:N:4022:HEM:HMC2	15:N:4022:HEM:HBC2	1.95	0.47
11:V:75:ILE:CG2	11:V:76:SER:H	2.18	0.47
2:B:317:ALA:O	2:B:321:THR:HG22	2.15	0.47
3:C:208:ASN:HD22	3:C:210:LEU:N	2.09	0.47
7:G:45:PHE:O	7:G:48:LEU:HB2	2.15	0.47
10:J:61:ASN:HD22	10:J:61:ASN:C	2.23	0.47
1:L:72:LEU:HD22	1:L:188:LEU:HD23	1.97	0.47
2:M:233:PHE:HB3	2:M:357:GLY:HA2	1.97	0.47
4:O:225:MET:HB2	15:O:4023:HEM:C1D	2.49	0.47
3:C:95:MET:HE1	18:C:4031:CN6:H43A	1.97	0.47
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.79	0.47
4:D:69:LEU:HD12	4:D:217:TYR:CE2	2.49	0.47
4:D:92:ARG:O	4:D:96:VAL:HG23	2.15	0.47
4:D:125:VAL:HA	4:D:128:MET:HE3	1.97	0.47
3:N:17:ILE:HG23	3:N:226:ILE:HD11	1.97	0.47
2:B:271:ILE:HG22	2:B:289:VAL:HG22	1.97	0.47
3:C:323:LYS:NZ	8:H:55:GLN:HE22	2.13	0.47
2:M:152:ARG:O	2:M:153:LYS:HB2	2.14	0.47
4:O:123:GLU:CD	4:O:123:GLU:H	2.23	0.47
11:K:2:ILE:HG22	11:K:3:GLU:N	2.29	0.46
10:U:99:SER:HB3	10:U:109:MET:HG2	1.97	0.46
1:A:156:HIS:HD2	1:A:159:ARG:NH2	2.13	0.46
1:A:292:GLU:CD	2:B:53:ARG:HH12	2.23	0.46
5:P:106:ASN:ND2	5:P:119:ARG:HH21	2.14	0.46
10:U:21:THR:HB	10:U:80:PHE:HD2	1.79	0.46
1:A:261:ILE:HG13	1:A:262:SER:N	2.29	0.46
10:J:20:LEU:HD12	10:J:81:LEU:HD23	1.97	0.46
2:B:43:THR:HG22	2:B:178:LYS:NZ	2.31	0.46
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.96	0.46
5:E:114:LYS:H	5:E:114:LYS:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:347:LYS:H	2:M:347:LYS:CD	2.07	0.46
10:U:37:TRP:CE2	10:U:81:LEU:HB2	2.50	0.46
12:W:70:GLU:CD	12:W:70:GLU:H	2.22	0.46
1:A:291:PHE:HZ	1:A:335:ARG:HH11	1.63	0.46
3:C:35:LEU:HD13	23:C:5040:HOH:O	2.15	0.46
3:C:99:LYS:HD2	3:C:99:LYS:C	2.40	0.46
4:D:256:ASN:C	4:D:256:ASN:HD22	2.23	0.46
5:E:146:ARG:NH2	5:E:202:ILE:HD11	2.31	0.46
8:H:3:PRO:HG3	8:S:12:TRP:CZ2	2.49	0.46
1:L:252:ARG:HD2	8:S:21:GLN:HB2	1.96	0.46
4:D:286:TRP:CZ3	5:E:56:ALA:HA	2.51	0.46
1:L:109:LEU:HB3	1:L:110:PRO:HD2	1.97	0.46
1:A:37:VAL:HG13	1:A:207:VAL:HA	1.97	0.46
16:C:4005:SMA:H39	16:C:4005:SMA:H33	1.97	0.46
2:B:251:ALA:HB2	2:B:339:ASN:HB3	1.97	0.46
7:G:43:LEU:HD21	7:G:78:ALA:HB1	1.97	0.46
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.55	0.46
1:A:270:VAL:HG21	1:A:396:ILE:HD13	1.98	0.46
2:B:315:SER:HB2	2:B:318:ILE:HD13	1.96	0.46
4:D:109:ARG:HG3	4:D:178:SER:HB2	1.98	0.46
5:E:44:LYS:HZ2	5:E:52:GLY:H	1.61	0.46
6:Q:87:ASN:O	6:Q:92:LYS:HE2	2.15	0.46
1:A:102:GLN:HE22	1:A:196:PHE:HE1	1.63	0.46
2:B:146:LEU:O	2:B:150:THR:HG23	2.16	0.46
4:D:223:ILE:HG12	4:D:225:MET:H	1.79	0.46
11:K:37:GLN:O	11:K:44:ILE:HA	2.16	0.46
4:O:256:ASN:C	4:O:256:ASN:HD22	2.24	0.46
4:O:286:TRP:CZ3	5:P:56:ALA:HA	2.50	0.46
3:C:263:LEU:HD22	5:P:115:PRO:HB3	1.98	0.45
4:D:277:LEU:HD21	20:D:4014:7PH:H33A	1.99	0.45
5:E:55:TYR:O	5:E:59:MET:HG2	2.16	0.45
5:E:213:ILE:O	5:E:213:ILE:HG12	2.16	0.45
2:M:30:THR:HG21	2:M:90:LYS:HE2	1.98	0.45
4:O:268:ARG:NH1	9:T:33:ASP:OD1	2.49	0.45
5:P:51:LYS:HE2	5:P:55:TYR:HE1	1.81	0.45
10:U:36:ASN:OD1	10:U:51:TYR:HB3	2.16	0.45
2:B:53:ARG:HB3	2:B:123:VAL:HG13	1.98	0.45
2:B:331:SER:C	2:B:333:SER:H	2.24	0.45
1:L:130:ASN:N	1:L:130:ASN:ND2	2.64	0.45
1:A:57:SER:HA	1:A:61:ASN:ND2	2.30	0.45
2:B:52:ASN:HD21	2:B:80:SER:C	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:ARG:HD3	2:B:224:PHE:CD1	2.52	0.45
7:G:53:ASN:ND2	7:G:56:MET:H	2.13	0.45
10:J:99:SER:HA	10:J:109:MET:HA	1.97	0.45
1:L:130:ASN:HD22	1:L:130:ASN:H	1.63	0.45
1:L:181:THR:O	1:L:185:LEU:HB2	2.17	0.45
5:P:146:ARG:CZ	5:P:202:ILE:HD11	2.46	0.45
2:B:141:SER:O	2:B:145:GLN:HG2	2.16	0.45
2:B:313:ASP:HB3	2:B:344:LYS:O	2.16	0.45
4:D:113:ARG:HG2	4:D:151:LEU:O	2.17	0.45
11:K:93:LYS:NZ	11:K:93:LYS:HB3	2.31	0.45
10:U:87:THR:HG22	10:U:88:THR:N	2.30	0.45
14:A:4021:UMQ:HC1	9:I:18:VAL:HG12	1.97	0.45
5:E:38:ASN:HD21	5:E:40:ASP:CG	2.24	0.45
7:G:41:LEU:HB2	7:G:43:LEU:HD23	1.99	0.45
1:L:88:LYS:HG3	2:M:264:LEU:HD21	1.99	0.45
5:E:100:ALA:O	5:E:102:PRO:HD3	2.17	0.45
6:F:94:LEU:HB3	6:F:130:LEU:HD23	1.98	0.45
11:K:13:ALA:O	11:K:106:ILE:HG22	2.16	0.45
3:N:313:VAL:HG22	3:N:319:LYS:HE3	1.99	0.45
11:V:93:LYS:HZ3	11:V:94:PHE:N	2.08	0.45
1:A:74:LYS:HG3	1:A:95:SER:HB3	1.98	0.45
2:M:251:ALA:HB2	2:M:339:ASN:HB3	1.99	0.45
4:O:134:TYR:OH	4:O:156:PRO:HD3	2.17	0.45
2:M:289:VAL:HG12	2:M:297:VAL:HG13	1.99	0.45
1:A:239:LYS:HB2	1:A:240:LYS:H	1.54	0.45
7:G:26:VAL:HG12	7:G:30:ASN:ND2	2.31	0.45
10:J:91:THR:HG23	10:J:119:THR:HA	1.98	0.45
2:M:251:ALA:O	2:M:255:VAL:HG13	2.16	0.45
10:U:21:THR:HB	10:U:80:PHE:CD2	2.52	0.45
1:A:382:ASN:HA	1:A:383:PRO:HD3	1.78	0.45
4:D:147:ARG:NH2	4:D:150:LYS:HE3	2.32	0.45
5:E:120:HIS:ND1	5:E:152:TRP:CH2	2.85	0.45
10:J:37:TRP:CE2	10:J:81:LEU:HB2	2.53	0.45
2:M:205:LEU:HD12	2:M:205:LEU:H	1.82	0.45
7:R:5:PHE:CD1	7:R:107:ILE:HG21	2.52	0.45
11:V:32:PHE:N	11:V:32:PHE:CD2	2.84	0.45
1:A:66:ASN:HD22	1:A:66:ASN:N	2.06	0.44
2:B:265:SER:C	2:B:267:LEU:H	2.25	0.44
1:L:289:ASN:C	1:L:289:ASN:HD22	2.25	0.44
2:M:246:ASN:ND2	2:M:246:ASN:N	2.63	0.44
2:M:262:SER:HB3	2:M:320:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:82:LYS:HE2	10:U:84:ASN:OD1	2.16	0.44
11:V:60:SER:C	11:V:62:PHE:H	2.25	0.44
11:K:29:ILE:HA	11:K:92:ILE:HG21	1.99	0.44
1:L:97:ILE:HD13	1:L:102:GLN:HG3	1.98	0.44
12:W:57:TYR:CD1	12:W:61:ASN:ND2	2.85	0.44
1:A:73:TRP:CZ3	1:A:76:ILE:HD11	2.53	0.44
1:A:234:THR:HG22	1:A:235:LYS:N	2.32	0.44
1:L:230:LEU:O	1:L:231:GLN:HB2	2.16	0.44
1:A:280:LEU:HD23	1:A:280:LEU:C	2.42	0.44
6:F:104:ARG:HG2	6:F:108:GLN:HE21	1.82	0.44
11:K:39:LYS:NZ	11:K:81:GLU:HG2	2.32	0.44
1:A:76:ILE:CG2	1:A:140:THR:HG21	2.47	0.44
2:B:215:LEU:HB2	23:B:7003:HOH:O	2.16	0.44
3:C:104:GLY:O	3:C:107:ARG:HG2	2.18	0.44
4:D:227:ARG:NH1	4:D:244:THR:HG21	2.33	0.44
7:G:97:GLN:H	7:G:97:GLN:NE2	2.15	0.44
1:L:302:LEU:HB2	1:L:350:GLN:HG3	2.00	0.44
1:A:62:GLU:OE1	1:A:67:ASN:HA	2.18	0.44
2:B:145:GLN:OE1	2:B:229:ASN:ND2	2.49	0.44
10:J:12:VAL:O	10:J:120:VAL:HA	2.18	0.44
2:M:205:LEU:HD12	2:M:205:LEU:N	2.33	0.44
10:U:34:TYR:HB2	10:U:99:SER:OG	2.18	0.44
3:C:32:MET:HE1	18:C:4031:CN6:H43	1.99	0.44
5:E:134:MET:HG2	23:J:7001:HOH:O	2.16	0.44
7:G:18:SER:OG	7:G:21:LEU:HD23	2.18	0.44
4:O:111:ALA:HA	4:O:154:TYR:HA	2.00	0.44
1:A:88:LYS:HE3	2:B:264:LEU:HD22	2.00	0.44
1:A:109:LEU:HB3	1:A:110:PRO:HD2	2.00	0.44
1:A:127:GLN:HA	1:A:130:ASN:HD22	1.82	0.44
1:A:141:LYS:HE3	1:A:186:GLU:HA	2.00	0.44
7:G:120:LEU:O	7:G:123:ILE:HG12	2.18	0.44
1:A:160:VAL:HG21	1:A:436:THR:HG22	1.99	0.43
2:B:232:ARG:NH1	2:M:164:VAL:CG2	2.81	0.43
1:L:429:GLN:HE22	9:T:13:ARG:NH2	2.16	0.43
3:C:150:LEU:HD21	3:C:295:MET:HE1	1.99	0.43
3:C:157:VAL:O	3:C:161:ILE:HG12	2.18	0.43
11:V:32:PHE:N	11:V:32:PHE:HD2	2.15	0.43
1:A:248:GLU:HA	1:A:433:ILE:O	2.19	0.43
2:M:220:GLU:HA	2:M:221:PRO:HD3	1.83	0.43
4:O:76:TRP:CZ2	4:O:188:CYS:HB3	2.53	0.43
2:B:314:LEU:C	2:B:316:PRO:HD3	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:TYR:CE1	3:C:248:PRO:HB2	2.53	0.43
2:M:56:PHE:CZ	2:M:78:PHE:HB3	2.53	0.43
3:N:125:ILE:HG22	16:N:4025:SMA:H37	2.00	0.43
5:P:107:VAL:CG1	5:P:118:ILE:HB	2.48	0.43
2:B:43:THR:HG22	2:B:178:LYS:HZ3	1.83	0.43
2:B:220:GLU:HA	2:B:221:PRO:HD3	1.84	0.43
2:B:250:LEU:HD21	2:B:336:ILE:HD13	2.00	0.43
1:L:311:LEU:HB3	1:L:343:LEU:HG	2.00	0.43
8:S:3:PRO:HA	8:S:4:PRO:HD3	1.86	0.43
10:U:54:ASN:C	10:U:72:ARG:HH22	2.27	0.43
10:U:65:LYS:HA	10:U:68:LEU:HD11	2.00	0.43
5:E:132:VAL:HG21	5:E:192:ARG:NH1	2.34	0.43
5:P:93:LYS:HG2	5:P:213:ILE:HD11	2.00	0.43
10:U:49:VAL:HG12	10:U:68:LEU:HD23	2.01	0.43
3:C:315:GLY:HA3	23:C:6558:HOH:O	2.17	0.43
11:K:8:PRO:O	11:K:102:THR:HG23	2.19	0.43
2:M:204:SER:OG	2:M:206:LEU:HB2	2.18	0.43
3:N:253:HIS:HE1	3:N:268:SER:O	2.01	0.43
7:R:63:LEU:HD12	7:R:64:PRO:HD2	2.00	0.43
10:U:61:ASN:ND2	10:U:63:SER:H	2.12	0.43
1:A:366:ALA:O	1:A:370:LEU:HB2	2.18	0.43
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.51	0.43
18:C:4031:CN6:H3A	18:C:4031:CN6:H57	1.65	0.43
5:E:44:LYS:HZ3	5:E:52:GLY:H	1.64	0.43
1:A:43:ASN:HA	1:A:44:PRO:HD2	1.85	0.43
4:D:187:GLY:O	4:D:191:ILE:HG12	2.19	0.43
10:J:41:PHE:HB3	10:J:42:PRO:HD2	2.00	0.43
1:L:169:PHE:O	1:L:172:THR:HB	2.18	0.43
5:P:181:HIS:HB2	21:P:4024:FES:S1	2.58	0.43
7:G:39:LYS:HG2	7:G:94:ILE:HB	2.00	0.43
11:K:103:LYS:HG2	11:K:104:LEU:N	2.34	0.43
2:B:42:ALA:HB1	2:B:47:VAL:HG12	2.01	0.42
2:B:121:GLU:OE2	7:R:62:ARG:HD2	2.19	0.42
3:C:216:LEU:HD12	3:C:216:LEU:N	2.33	0.42
1:L:74:LYS:HG3	1:L:95:SER:CB	2.49	0.42
2:M:49:HIS:HE1	2:M:130:ASP:OD1	2.02	0.42
4:O:86:ASP:HA	9:T:47:LYS:HG2	2.00	0.42
2:B:30:THR:CG2	2:B:190:GLU:HB3	2.46	0.42
1:L:207:VAL:HG21	1:L:394:VAL:HG23	2.00	0.42
10:J:98:ARG:O	10:J:109:MET:HA	2.19	0.42
11:K:7:THR:HG23	11:K:22:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:17:ASP:HB2	11:K:18:ARG:NH2	2.34	0.42
1:L:401:LEU:HB3	23:L:7297:HOH:O	2.18	0.42
2:M:251:ALA:CB	2:M:339:ASN:HB3	2.49	0.42
3:N:138:GLN:OE1	3:N:138:GLN:HA	2.20	0.42
5:P:93:LYS:HG3	5:P:214:VAL:O	2.18	0.42
10:U:12:VAL:O	10:U:120:VAL:HA	2.19	0.42
10:U:34:TYR:HB2	10:U:99:SER:HG	1.84	0.42
1:A:76:ILE:HG23	1:A:140:THR:HG21	2.01	0.42
1:L:42:HIS:HB2	23:L:7033:HOH:O	2.18	0.42
2:M:254:GLU:CG	2:M:278:LYS:HE3	2.50	0.42
2:B:117:HIS:HB3	7:R:62:ARG:HG2	2.02	0.42
2:B:270:LEU:HB3	2:B:304:ILE:HD11	2.01	0.42
11:K:79:GLU:HA	11:K:80:PRO:HA	1.74	0.42
4:D:111:ALA:HA	4:D:154:TYR:HA	2.01	0.42
7:G:62:ARG:HG2	2:M:117:HIS:HB3	2.01	0.42
10:J:38:ILE:HA	10:J:49:VAL:HG23	2.01	0.42
1:L:386:ASP:O	1:L:390:LEU:HB2	2.20	0.42
2:M:347:LYS:CG	2:M:348:LEU:H	2.23	0.42
4:D:147:ARG:HG2	4:D:148:PRO:O	2.20	0.42
8:H:61:ILE:O	8:H:65:ILE:HG13	2.20	0.42
11:K:4:LEU:CD2	11:K:88:CYS:SG	3.08	0.42
1:L:58:GLY:H	1:L:61:ASN:ND2	2.10	0.42
1:L:169:PHE:CD1	1:L:174:LEU:HB3	2.55	0.42
3:N:216:LEU:N	3:N:216:LEU:HD12	2.35	0.42
12:W:18:LEU:HD23	12:W:103:LEU:HB2	2.02	0.42
1:A:386:ASP:O	1:A:390:LEU:HB2	2.19	0.42
1:L:447:ARG:NH1	3:N:18:ILE:HG22	2.34	0.42
6:Q:81:LEU:HB3	6:Q:138:THR:HG22	2.02	0.42
1:A:344:ILE:HG21	1:A:448:ILE:HD12	2.02	0.42
2:B:332:VAL:O	2:B:332:VAL:HG12	2.20	0.42
5:P:120:HIS:ND1	5:P:152:TRP:CH2	2.87	0.42
7:R:115:LYS:HE3	7:R:119:GLU:OE2	2.20	0.42
10:U:6:GLU:HG2	10:U:96:CYS:SG	2.60	0.42
2:B:39:SER:OG	2:B:84:ARG:HA	2.20	0.41
2:M:338:LEU:H	2:M:338:LEU:HD22	1.84	0.41
3:N:77:ILE:O	3:N:81:LEU:HB2	2.19	0.41
2:B:66:LYS:HE3	2:B:70:GLU:OE2	2.20	0.41
18:C:4031:CN6:HAA	7:G:85:HIS:CE1	2.55	0.41
4:D:76:TRP:CZ2	4:D:188:CYS:HB3	2.55	0.41
5:E:125:GLU:HB3	5:E:187:ILE:HG12	2.02	0.41
11:K:19:VAL:HG12	11:K:75:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:44:LYS:HB2	2:M:47:VAL:CG2	2.50	0.41
18:N:4131:CN6:H3A	18:N:4131:CN6:H57	1.81	0.41
10:U:36:ASN:HD21	10:U:99:SER:CB	2.33	0.41
2:B:53:ARG:HD3	2:B:130:ASP:OD1	2.19	0.41
5:E:165:VAL:HG23	3:N:142:TRP:CH2	2.55	0.41
11:K:46:LEU:HD23	11:K:55:HIS:CD2	2.54	0.41
3:N:139:MET:HE3	3:N:255:ASP:HB3	2.02	0.41
2:B:98:LEU:O	2:B:102:VAL:HG23	2.20	0.41
3:C:313:VAL:CG2	3:C:319:LYS:HE3	2.50	0.41
1:L:315:PHE:CD1	1:L:315:PHE:C	2.98	0.41
1:A:447:ARG:NH1	3:C:18:ILE:HG22	2.36	0.41
7:G:91:ASN:H	7:G:91:ASN:HD22	1.69	0.41
11:K:48:ILE:HD13	11:K:54:LEU:HA	2.02	0.41
1:L:102:GLN:HE21	1:L:102:GLN:HB2	1.68	0.41
14:L:4121:UMQ:HC1	9:T:18:VAL:HG13	2.02	0.41
7:R:46:ASP:HB2	7:R:102:TYR:CE2	2.55	0.41
11:V:4:LEU:HD23	11:V:88:CYS:SG	2.61	0.41
2:B:183:GLU:HG2	2:B:211:ALA:HB1	2.03	0.41
7:G:127:LYS:HD3	7:G:127:LYS:N	2.36	0.41
1:L:379:GLU:OE1	2:M:26:THR:HB	2.21	0.41
1:A:220:VAL:O	1:A:224:GLU:HB2	2.21	0.41
10:J:29:ILE:H	10:J:77:ASN:HD21	1.69	0.41
11:K:58:VAL:HA	11:K:59:PRO:HD3	1.86	0.41
2:M:230:ARG:HH21	2:M:230:ARG:HG2	1.86	0.41
3:N:58:ILE:HD11	3:N:136:TYR:CZ	2.55	0.41
3:N:107:ARG:NH1	3:N:311:SER:O	2.54	0.41
10:U:61:ASN:HD22	10:U:61:ASN:C	2.28	0.41
1:A:252:ARG:HG3	1:A:439:ILE:HG13	2.02	0.41
1:A:364:GLU:HG3	7:R:125:VAL:HG21	2.03	0.41
3:C:178:ARG:HE	3:C:178:ARG:HB3	1.72	0.41
3:C:193:MET:CE	3:C:196:MET:SD	3.09	0.41
12:W:58:THR:HB	15:W:4026:HEM:O2D	2.20	0.41
1:A:179:ARG:HG2	1:A:179:ARG:NH2	2.35	0.41
1:A:266:GLU:O	1:A:425:ARG:HG3	2.21	0.41
2:B:31:LEU:HD21	2:B:197:LEU:HD11	2.03	0.41
2:B:41:TYR:HD2	2:B:215:LEU:HD13	1.86	0.41
2:B:46:GLY:HA3	2:B:161:TYR:HA	2.03	0.41
18:C:4031:CN6:H52A	18:C:4031:CN6:H2'	1.68	0.41
4:D:92:ARG:HG2	4:D:236:TYR:CE2	2.56	0.41
10:J:87:THR:HG22	10:J:89:GLU:H	1.85	0.41
1:L:43:ASN:HA	1:L:44:PRO:HD2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:72:LEU:HD13	1:L:144:VAL:HG21	2.03	0.41
2:M:39:SER:OG	2:M:84:ARG:HA	2.20	0.41
2:M:193:VAL:HG23	2:M:196:ASP:HB2	2.02	0.41
1:A:74:LYS:HE3	1:A:95:SER:O	2.21	0.41
2:B:309:LYS:C	2:B:311:GLY:H	2.29	0.41
3:C:234:PHE:CE2	4:D:280:LEU:HG	2.55	0.41
8:H:48:SER:O	8:H:49:PHE:HB2	2.21	0.41
1:L:318:PHE:HB2	1:L:320:LEU:HD13	2.03	0.41
3:N:314:ARG:HD3	23:N:5535:HOH:O	2.20	0.41
11:V:34:ASN:ND2	11:V:49:TYR:HA	2.36	0.41
12:W:43:GLY:N	12:W:111:ALA:O	2.53	0.41
4:D:123:GLU:CD	4:D:123:GLU:H	2.29	0.40
1:L:74:LYS:HB2	1:L:97:ILE:HD11	2.04	0.40
1:A:289:ASN:C	1:A:289:ASN:ND2	2.79	0.40
2:B:336:ILE:HD12	2:B:336:ILE:N	2.30	0.40
5:E:114:LYS:HD3	5:E:114:LYS:N	2.36	0.40
5:E:164:CYS:HB2	5:E:178:CYS:SG	2.62	0.40
8:H:3:PRO:HG3	8:S:12:TRP:CE2	2.56	0.40
10:J:51:TYR:C	10:J:51:TYR:HD2	2.29	0.40
3:N:323:LYS:HZ3	8:S:55:GLN:HE22	1.70	0.40
12:W:37:VAL:O	15:W:4026:HEM:HMD3	2.22	0.40
2:B:146:LEU:HD13	2:B:146:LEU:HA	1.93	0.40
1:L:46:ALA:HB3	1:L:213:ASN:HB3	2.03	0.40
4:O:212:SER:O	13:X:2:FRU:H4	2.22	0.40
4:O:273:THR:OG1	20:O:4114:7PH:H2	2.22	0.40
7:R:43:LEU:HD21	7:R:78:ALA:CB	2.51	0.40
2:B:364:TYR:CE1	2:M:152:ARG:HG2	2.56	0.40
10:J:10:GLY:HA2	10:J:118:VAL:HG12	2.02	0.40
11:K:4:LEU:HD21	11:K:33:LEU:HD11	2.04	0.40
8:S:88:GLU:O	8:S:92:VAL:HG22	2.20	0.40
10:U:29:ILE:N	10:U:77:ASN:HD21	2.06	0.40
12:W:96:LYS:HD3	12:W:98:LYS:HZ3	1.85	0.40
1:A:271:ASN:HD21	1:A:397:LYS:NZ	2.20	0.40
2:B:30:THR:OG1	2:B:90:LYS:HE3	2.22	0.40
2:B:145:GLN:HB3	2:B:354:VAL:HG11	2.03	0.40
3:C:20:SER:HA	3:C:21:PRO:HD3	1.91	0.40
10:U:54:ASN:H	10:U:54:ASN:ND2	2.18	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%)	395 (92%)	33 (8%)	1 (0%)	43	63
1	L	429/431 (100%)	393 (92%)	32 (8%)	4 (1%)	14	27
2	B	350/352 (99%)	310 (89%)	31 (9%)	9 (3%)	4	7
2	M	350/352 (99%)	320 (91%)	19 (5%)	11 (3%)	3	5
3	C	383/385 (100%)	364 (95%)	17 (4%)	2 (0%)	24	43
3	N	383/385 (100%)	367 (96%)	14 (4%)	2 (0%)	24	43
4	D	244/248 (98%)	231 (95%)	12 (5%)	1 (0%)	30	49
4	O	244/248 (98%)	234 (96%)	10 (4%)	0	100	100
5	E	183/185 (99%)	171 (93%)	9 (5%)	3 (2%)	7	14
5	P	183/185 (99%)	171 (93%)	10 (6%)	2 (1%)	11	22
6	F	72/146 (49%)	68 (94%)	4 (6%)	0	100	100
6	Q	72/146 (49%)	67 (93%)	4 (6%)	1 (1%)	9	17
7	G	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
7	R	123/126 (98%)	119 (97%)	4 (3%)	0	100	100
8	H	91/93 (98%)	78 (86%)	10 (11%)	3 (3%)	3	4
8	S	91/93 (98%)	82 (90%)	6 (7%)	3 (3%)	3	4
9	I	53/65 (82%)	48 (91%)	4 (8%)	1 (2%)	6	11
9	T	53/65 (82%)	50 (94%)	1 (2%)	2 (4%)	2	3
10	J	125/127 (98%)	110 (88%)	14 (11%)	1 (1%)	16	31
10	U	125/127 (98%)	110 (88%)	12 (10%)	3 (2%)	4	8
11	K	105/107 (98%)	80 (76%)	21 (20%)	4 (4%)	2	3
11	V	105/107 (98%)	82 (78%)	20 (19%)	3 (3%)	3	5
12	W	110/112 (98%)	98 (89%)	11 (10%)	1 (1%)	14	27
All	All	4426/4642 (95%)	4069 (92%)	300 (7%)	57 (1%)	9	18

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	152	ARG
2	B	153	LYS
2	B	335	PRO
2	B	343	VAL
3	C	346	VAL
8	H	37	LEU
8	H	93	ASN
11	K	80	PRO
2	M	153	LYS
2	M	335	PRO
2	M	343	VAL
2	M	348	LEU
5	P	103	LEU
2	B	214	SER
2	B	311	GLY
2	B	327	VAL
3	C	223	SER
5	E	102	PRO
5	E	103	LEU
8	H	36	PRO
10	J	65	LYS
1	L	126	GLN
2	M	311	GLY
2	M	338	LEU
3	N	223	SER
6	Q	118	GLU
8	S	37	LEU
2	B	338	LEU
5	E	46	ASN
9	I	55	ARG
11	K	51	THR
1	L	227	ASN
2	M	313	ASP
5	P	102	PRO
9	T	12	LYS
9	T	13	ARG
10	U	44	ASN
11	V	30	ASN
1	L	228	LEU
2	M	95	LYS
8	S	93	ASN
10	U	32	GLY

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Mol	Chain	Res	Type
12	W	6	GLY
1	A	127	GLN
4	D	263	HIS
11	K	10	SER
2	M	315	SER
2	M	327	VAL
8	S	36	PRO
10	U	15	SER
11	K	16	GLY
1	L	231	GLN
2	M	314	LEU
3	N	346	VAL
11	V	68	GLY
2	B	332	VAL
11	V	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%)	338 (91%)	32 (9%)	10	21
1	L	370/370 (100%)	338 (91%)	32 (9%)	10	21
2	B	301/301 (100%)	272 (90%)	29 (10%)	8	17
2	M	301/301 (100%)	269 (89%)	32 (11%)	6	14
3	C	338/338 (100%)	318 (94%)	20 (6%)	18	37
3	N	338/338 (100%)	321 (95%)	17 (5%)	22	44
4	D	204/206 (99%)	194 (95%)	10 (5%)	22	45
4	O	204/206 (99%)	194 (95%)	10 (5%)	22	45
5	E	151/151 (100%)	145 (96%)	6 (4%)	28	54
5	P	151/151 (100%)	146 (97%)	5 (3%)	33	61
6	F	67/130 (52%)	63 (94%)	4 (6%)	17	36
6	Q	67/130 (52%)	62 (92%)	5 (8%)	12	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	109/110 (99%)	102 (94%)	7 (6%)	16	33
7	R	109/110 (99%)	102 (94%)	7 (6%)	16	33
8	H	77/77 (100%)	76 (99%)	1 (1%)	61	82
8	S	77/77 (100%)	74 (96%)	3 (4%)	28	55
9	I	45/53 (85%)	44 (98%)	1 (2%)	45	73
9	T	45/53 (85%)	43 (96%)	2 (4%)	25	50
10	J	112/112 (100%)	105 (94%)	7 (6%)	16	34
10	U	112/112 (100%)	104 (93%)	8 (7%)	13	29
11	K	93/93 (100%)	86 (92%)	7 (8%)	12	26
11	V	93/93 (100%)	87 (94%)	6 (6%)	15	32
12	W	92/91 (101%)	86 (94%)	6 (6%)	15	32
All	All	3826/3973 (96%)	3569 (93%)	257 (7%)	15	31

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	66	ASN
1	A	113	THR
1	A	120	LEU
1	A	164	LEU
1	A	172	THR
1	A	185	LEU
1	A	188	LEU
1	A	193	LEU
1	A	203	ASN
1	A	208	VAL
1	A	237	VAL
1	A	239	LYS
1	A	252	ARG
1	A	261	ILE
1	A	271	ASN
1	A	272	SER
1	A	289	ASN
1	A	311	LEU
1	A	320	LEU
1	A	343	LEU
1	A	361	THR

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Mol	Chain	Res	Type
1	A	370	LEU
1	A	377	LEU
1	A	384	VAL
1	A	390	LEU
1	A	393	GLU
1	A	425	ARG
1	A	426	LEU
1	A	429	GLN
1	A	443	LEU
1	A	456	ARG
2	B	17	LEU
2	B	30	THR
2	B	31	LEU
2	B	53	ARG
2	B	54	PHE
2	B	62	ARG
2	B	73	LEU
2	B	136	GLN
2	B	144	ASP
2	B	146	LEU
2	B	150	THR
2	B	155	LEU
2	B	166	ARG
2	B	169	LEU
2	B	206	LEU
2	B	215	LEU
2	B	218	LYS
2	B	250	LEU
2	B	254	GLU
2	B	255	VAL
2	B	270	LEU
2	B	271	ILE
2	B	309	LYS
2	B	323	LEU
2	B	330	GLU
2	B	339	ASN
2	B	343	VAL
2	B	347	LYS
2	B	362	LEU
3	C	35	LEU
3	C	38	LEU
3	C	79	ARG

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Mol	Chain	Res	Type
3	C	99	LYS
3	C	107	ARG
3	C	111	VAL
3	C	150	LEU
3	C	175	THR
3	C	182	LEU
3	C	185	LEU
3	C	238	LEU
3	C	247	SER
3	C	292	VAL
3	C	302	LEU
3	C	312	VAL
3	C	313	VAL
3	C	335	LEU
3	C	336	LEU
3	C	350	LEU
3	C	377	LEU
4	D	69	LEU
4	D	109	ARG
4	D	113	ARG
4	D	115	LEU
4	D	141	GLN
4	D	251	VAL
4	D	256	ASN
4	D	280	LEU
4	D	283	LEU
4	D	288	LYS
5	E	42	VAL
5	E	51	LYS
5	E	114	LYS
5	E	206	GLU
5	E	211	LYS
5	E	213	ILE
6	F	77	GLN
6	F	89	GLU
6	F	94	LEU
6	F	130	LEU
7	G	16	LEU
7	G	48	LEU
7	G	58	THR
7	G	62	ARG
7	G	77	ARG

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Mol	Chain	Res	Type
7	G	123	ILE
7	G	127	LYS
8	H	60	LEU
9	I	18	VAL
10	J	38	ILE
10	J	39	ARG
10	J	44	ASN
10	J	51	TYR
10	J	61	ASN
10	J	68	LEU
10	J	114	GLN
11	K	7	THR
11	K	18	ARG
11	K	33	LEU
11	K	44	ILE
11	K	81	GLU
11	K	92	ILE
11	K	93	LYS
1	L	30	THR
1	L	66	ASN
1	L	89	GLU
1	L	117	LEU
1	L	120	LEU
1	L	130	ASN
1	L	153	ASP
1	L	164	LEU
1	L	172	THR
1	L	174	LEU
1	L	176	LEU
1	L	185	LEU
1	L	188	LEU
1	L	218	ASP
1	L	237	VAL
1	L	238	LEU
1	L	239	LYS
1	L	241	LYS
1	L	261	ILE
1	L	293	PRO
1	L	311	LEU
1	L	320	LEU
1	L	330	PHE
1	L	343	LEU

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Mol	Chain	Res	Type
1	L	370	LEU
1	L	374	LEU
1	L	377	LEU
1	L	390	LEU
1	L	424	LYS
1	L	425	ARG
1	L	426	LEU
1	L	443	LEU
2	M	17	LEU
2	M	30	THR
2	M	31	LEU
2	M	40	ARG
2	M	53	ARG
2	M	54	PHE
2	M	62	ARG
2	M	73	LEU
2	M	111	LYS
2	M	144	ASP
2	M	146	LEU
2	M	166	ARG
2	M	169	LEU
2	M	186	GLU
2	M	206	LEU
2	M	238	VAL
2	M	245	VAL
2	M	246	ASN
2	M	250	LEU
2	M	254	GLU
2	M	255	VAL
2	M	271	ILE
2	M	310	LYS
2	M	312	LYS
2	M	318	ILE
2	M	323	LEU
2	M	324	LYS
2	M	329	ASN
2	M	330	GLU
2	M	345	ASP
2	M	347	LYS
2	M	362	LEU
3	N	35	LEU
3	N	38	LEU

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Mol	Chain	Res	Type
3	N	79	ARG
3	N	99	LYS
3	N	150	LEU
3	N	182	LEU
3	N	185	LEU
3	N	283	ARG
3	N	292	VAL
3	N	302	LEU
3	N	312	VAL
3	N	313	VAL
3	N	321	LEU
3	N	335	LEU
3	N	336	LEU
3	N	350	LEU
3	N	377	LEU
4	O	69	LEU
4	O	109	ARG
4	O	115	LEU
4	O	150	LYS
4	O	163	GLN
4	O	179	LEU
4	O	251	VAL
4	O	256	ASN
4	O	280	LEU
4	O	283	LEU
5	P	51	LYS
5	P	65	LEU
5	P	80	SER
5	P	110	LYS
5	P	211	LYS
6	Q	74	VAL
6	Q	77	GLN
6	Q	94	LEU
6	Q	95	VAL
6	Q	130	LEU
7	R	16	LEU
7	R	41	LEU
7	R	48	LEU
7	R	61	ARG
7	R	62	ARG
7	R	125	VAL
7	R	127	LYS

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Mol	Chain	Res	Type
8	S	35	LYS
8	S	60	LEU
8	S	68	TYR
9	T	14	ASN
9	T	18	VAL
10	U	3	LYS
10	U	21	THR
10	U	38	ILE
10	U	39	ARG
10	U	59	ASN
10	U	61	ASN
10	U	66	ASP
10	U	68	LEU
11	V	18	ARG
11	V	81	GLU
11	V	89	GLN
11	V	92	ILE
11	V	93	LYS
11	V	104	LEU
12	W	2	LYS
12	W	51	GLN
12	W	53	LYS
12	W	58	THR
12	W	82	LYS
12	W	89	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	66	ASN
1	A	67	ASN
1	A	96	ASN
1	A	102	GLN
1	A	126	GLN
1	A	130	ASN
1	A	154	ASN
1	A	156	HIS
1	A	170	GLN
1	A	198	ASN
1	A	231	GLN
1	A	271	ASN

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Mol	Chain	Res	Type
1	A	274	ASN
1	A	289	ASN
1	A	314	ASN
1	A	317	HIS
1	A	336	ASN
1	A	350	GLN
1	A	376	GLN
1	A	382	ASN
1	A	385	ASN
1	A	388	ASN
1	A	429	GLN
2	B	49	HIS
2	B	52	ASN
2	B	55	ASN
2	B	57	GLN
2	B	103	ASN
2	B	246	ASN
2	B	252	GLN
2	B	339	ASN
3	C	14	ASN
3	C	22	GLN
3	C	43	GLN
3	C	74	ASN
3	C	173	ASN
3	C	202	HIS
3	C	208	ASN
3	C	253	HIS
3	C	332	ASN
3	C	384	ASN
4	D	78	HIS
4	D	79	ASN
4	D	127	ASN
4	D	256	ASN
4	D	303	ASN
5	E	38	ASN
5	E	46	ASN
5	E	97	ASN
5	E	106	ASN
5	E	184	HIS
6	F	77	GLN
6	F	84	HIS
6	F	108	GLN

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Mol	Chain	Res	Type
6	F	111	GLN
6	F	119	HIS
6	F	129	HIS
7	G	30	ASN
7	G	53	ASN
7	G	79	HIS
7	G	86	HIS
7	G	91	ASN
7	G	97	GLN
8	H	55	GLN
9	I	14	ASN
9	I	29	GLN
10	J	44	ASN
10	J	54	ASN
10	J	61	ASN
10	J	77	ASN
10	J	78	GLN
11	K	34	ASN
11	K	89	GLN
11	K	91	HIS
1	L	34	ASN
1	L	61	ASN
1	L	63	ASN
1	L	66	ASN
1	L	67	ASN
1	L	102	GLN
1	L	122	GLN
1	L	130	ASN
1	L	156	HIS
1	L	170	GLN
1	L	227	ASN
1	L	283	GLN
1	L	289	ASN
1	L	314	ASN
1	L	317	HIS
1	L	336	ASN
1	L	350	GLN
1	L	385	ASN
1	L	388	ASN
2	M	49	HIS
2	M	52	ASN
2	M	55	ASN

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Mol	Chain	Res	Type
2	M	57	GLN
2	M	246	ASN
2	M	252	GLN
2	M	258	ASN
2	M	329	ASN
2	M	339	ASN
2	M	361	ASN
3	N	14	ASN
3	N	22	GLN
3	N	57	ASN
3	N	74	ASN
3	N	208	ASN
3	N	253	HIS
4	O	78	HIS
4	O	79	ASN
4	O	127	ASN
4	O	163	GLN
4	O	256	ASN
5	P	38	ASN
5	P	97	ASN
5	P	106	ASN
5	P	112	GLN
5	P	127	GLN
5	P	130	ASN
5	P	184	HIS
6	Q	77	GLN
7	R	30	ASN
7	R	31	GLN
7	R	79	HIS
7	R	91	ASN
7	R	97	GLN
8	S	38	GLN
8	S	55	GLN
9	T	14	ASN
9	T	29	GLN
9	T	42	ASN
10	U	54	ASN
10	U	59	ASN
10	U	61	ASN
10	U	77	ASN
10	U	78	GLN
11	V	34	ASN

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Mol	Chain	Res	Type
11	V	38	GLN
11	V	77	ASN
11	V	90	HIS
11	V	91	HIS
12	W	101	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	81	12	10,11,12	0.86	0	9,14,16	1.23	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	81	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	81	M3L	CM3-NZ-CM1	-2.49	102.43	108.98

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	0.77	0	15,15,17	0.92	1 (6%)
13	FRU	X	2	13	11,12,12	0.72	1 (9%)	10,18,18	0.53	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	-	0/2/19/22	0/1/1/1
13	FRU	X	2	13	-	0/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	2	FRU	O2-C2	2.05	1.44	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X	1	GLC	C2-C3-C4	-2.96	105.66	110.86

There are no chirality outliers.

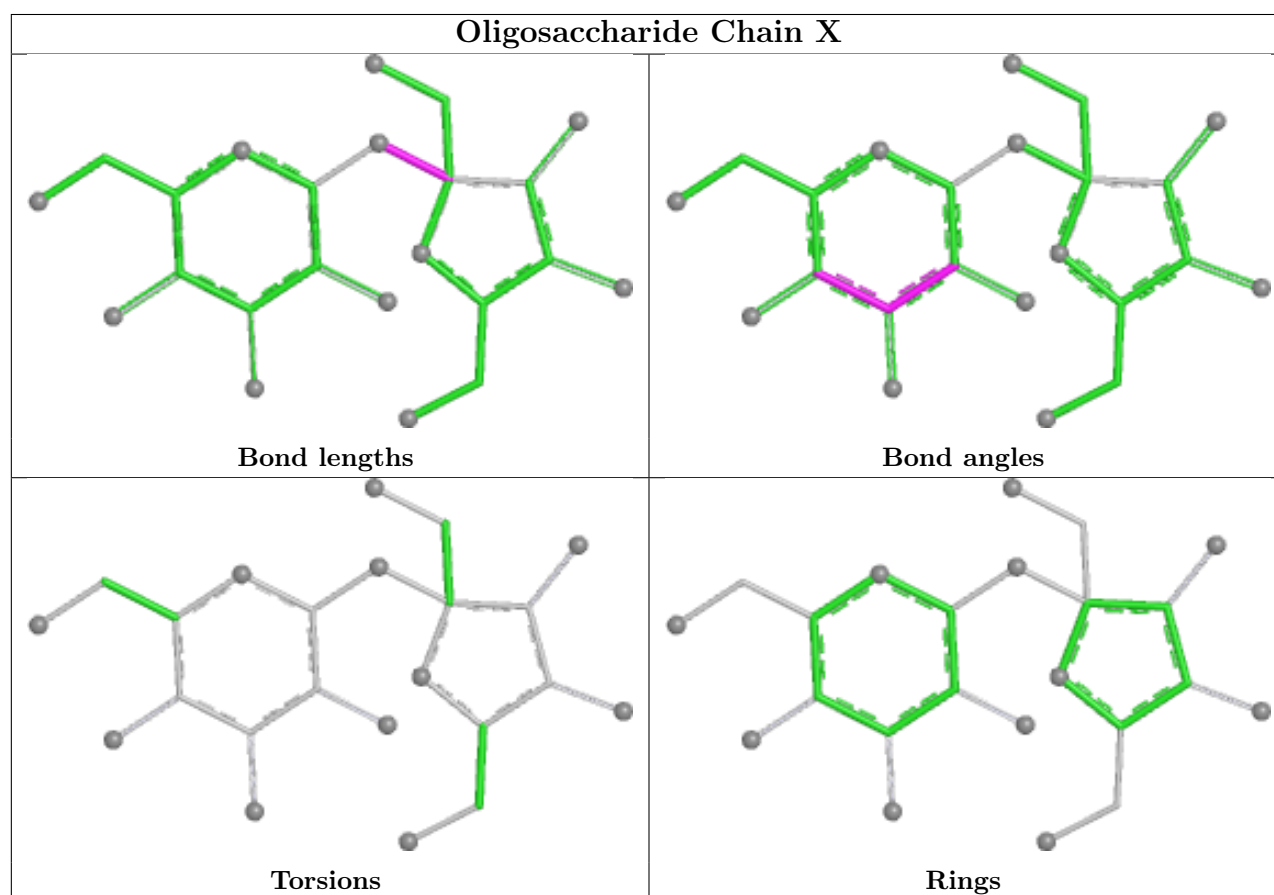
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

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



5.6 Ligand geometry [i](#)

23 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
15	HEM	W	4026	12	50,50,50	1.48	8 (16%)	67,82,82	1.06	5 (7%)
15	HEM	N	4022	3	50,50,50	1.28	6 (12%)	67,82,82	0.69	1 (1%)
20	7PH	O	4114	-	37,37,37	1.08	2 (5%)	40,42,42	1.49	9 (22%)
20	7PH	D	4014	-	37,37,37	1.07	2 (5%)	40,42,42	1.44	9 (22%)
14	UMQ	L	4121	-	35,35,35	1.00	1 (2%)	46,46,46	1.76	5 (10%)
17	8PE	N	4110	-	46,46,46	0.93	2 (4%)	49,51,51	1.19	3 (6%)
15	HEM	O	4023	4	50,50,50	1.45	4 (8%)	67,82,82	1.04	6 (8%)
19	9PE	N	4011	-	39,39,39	0.75	0	42,44,44	0.93	1 (2%)
21	FES	P	4024	5	0,4,4	-	-	-	-	-
19	9PE	C	4111	-	39,39,39	0.79	0	42,44,44	0.96	1 (2%)
15	HEM	C	4002	3	50,50,50	1.26	7 (14%)	67,82,82	0.68	0
15	HEM	D	4003	4	50,50,50	1.39	5 (10%)	67,82,82	1.11	5 (7%)
22	6PH	L	4113	-	39,39,39	0.99	2 (5%)	42,44,44	1.39	4 (9%)
22	6PH	E	4013	-	39,39,39	0.97	3 (7%)	42,44,44	1.36	4 (9%)
18	CN6	N	4131	-	49,49,49	1.67	10 (20%)	55,61,61	1.69	12 (21%)
18	CN6	C	4031	-	49,49,49	1.62	10 (20%)	55,61,61	1.56	10 (18%)
15	HEM	N	4021	3	50,50,50	1.30	8 (16%)	67,82,82	0.97	3 (4%)
17	8PE	C	4010	-	46,46,46	0.97	3 (6%)	49,51,51	1.03	1 (2%)
16	SMA	C	4005	-	38,38,38	1.05	2 (5%)	47,52,52	0.95	2 (4%)
14	UMQ	A	4021	-	35,35,35	0.99	2 (5%)	46,46,46	1.70	7 (15%)
15	HEM	C	4001	3	50,50,50	1.31	6 (12%)	67,82,82	0.96	3 (4%)
21	FES	E	4004	5	0,4,4	-	-	-	-	-
16	SMA	N	4025	-	38,38,38	1.02	3 (7%)	47,52,52	0.83	1 (2%)

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
15	HEM	W	4026	12	-	6/14/54/54	-
15	HEM	N	4022	3	-	5/14/54/54	-
20	7PH	O	4114	-	-	12/39/39/39	-
20	7PH	D	4014	-	-	14/39/39/39	-
14	UMQ	L	4121	-	-	4/20/60/60	0/2/2/2
17	8PE	N	4110	-	-	18/50/50/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HEM	O	4023	4	-	10/14/54/54	-
19	9PE	N	4011	-	-	22/43/43/43	-
21	FES	P	4024	5	-	-	0/1/1/1
19	9PE	C	4111	-	-	19/43/43/43	-
15	HEM	C	4002	3	-	4/14/54/54	-
15	HEM	D	4003	4	-	10/14/54/54	-
22	6PH	L	4113	-	-	20/41/41/41	-
22	6PH	E	4013	-	-	17/41/41/41	-
18	CN6	N	4131	-	-	27/60/60/60	-
18	CN6	C	4031	-	-	26/60/60/60	-
15	HEM	N	4021	3	-	6/14/54/54	-
17	8PE	C	4010	-	-	23/50/50/50	-
16	SMA	C	4005	-	-	2/34/34/34	0/2/2/2
14	UMQ	A	4021	-	-	4/20/60/60	0/2/2/2
15	HEM	C	4001	3	-	4/14/54/54	-
21	FES	E	4004	5	-	-	0/1/1/1
16	SMA	N	4025	-	-	1/34/34/34	0/2/2/2

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	4023	HEM	CBB-CAB	5.00	1.54	1.30
15	D	4003	HEM	CBC-CAC	4.85	1.53	1.30
15	W	4026	HEM	CBC-CAC	4.78	1.53	1.30
15	D	4003	HEM	CBB-CAB	4.74	1.53	1.30
15	O	4023	HEM	CBC-CAC	4.60	1.52	1.30
15	W	4026	HEM	CBB-CAB	4.56	1.52	1.30
18	N	4131	CN6	O31-C3	-4.35	1.35	1.45
18	C	4031	CN6	O31-C3	-4.28	1.35	1.45
14	L	4121	UMQ	C3-C2	-3.99	1.42	1.52
18	N	4131	CN6	O21-C2	-3.82	1.37	1.46
15	N	4022	HEM	CBC-CAC	3.80	1.48	1.30
18	C	4031	CN6	O21-C2	-3.79	1.37	1.46
20	D	4014	7PH	O31-C3	-3.68	1.36	1.45
20	O	4114	7PH	O31-C3	-3.68	1.36	1.45
15	N	4022	HEM	CMA-C3A	3.67	1.58	1.50
15	N	4021	HEM	CAC-C3C	-3.53	1.38	1.47
14	A	4021	UMQ	C3-C2	-3.52	1.43	1.52
15	C	4001	HEM	CAC-C3C	-3.51	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	4002	HEM	CBC-CAC	3.49	1.47	1.30
15	C	4001	HEM	CAB-C3B	-3.46	1.38	1.47
15	O	4023	HEM	FE-NB	3.46	2.05	1.94
18	C	4031	CN6	O3'-CA	-3.45	1.31	1.44
16	C	4005	SMA	C20-C19	3.40	1.36	1.33
18	N	4131	CN6	O3'-CA	-3.38	1.31	1.44
15	N	4021	HEM	CAB-C3B	-3.23	1.38	1.47
16	C	4005	SMA	O1-C2	3.20	1.40	1.36
15	C	4002	HEM	CBB-CAB	3.18	1.45	1.30
18	N	4131	CN6	CA-CB	3.17	1.61	1.51
15	C	4001	HEM	CMC-C2C	3.10	1.57	1.50
15	N	4022	HEM	FE-NA	3.06	2.05	1.95
16	N	4025	SMA	O1-C2	3.06	1.40	1.36
18	C	4031	CN6	CC-CB	3.06	1.61	1.51
15	W	4026	HEM	FE-NB	3.01	2.04	1.94
17	C	4010	8PE	O21-C21	3.01	1.42	1.34
15	N	4022	HEM	CAB-C3B	-3.00	1.39	1.47
18	N	4131	CN6	O32-C31	-2.99	1.13	1.22
15	N	4021	HEM	CBB-CAB	2.93	1.44	1.30
18	C	4031	CN6	O32-C31	-2.82	1.14	1.22
15	W	4026	HEM	FE-NA	2.79	2.04	1.95
15	C	4002	HEM	FE-NA	2.79	2.04	1.95
18	N	4131	CN6	CC-CB	2.79	1.60	1.51
16	N	4025	SMA	C8-C8A	2.77	1.44	1.39
15	W	4026	HEM	CAC-C3C	2.71	1.54	1.47
15	N	4021	HEM	CMC-C2C	2.71	1.56	1.50
15	C	4002	HEM	CAB-C3B	-2.69	1.40	1.47
18	C	4031	CN6	CA-CB	2.68	1.60	1.51
15	C	4001	HEM	CBC-CAC	2.66	1.43	1.30
15	D	4003	HEM	FE-ND	2.64	2.03	1.94
15	N	4022	HEM	CBB-CAB	2.61	1.42	1.30
15	N	4021	HEM	FE-NA	2.59	2.03	1.95
17	N	4110	8PE	O21-C21	2.58	1.41	1.34
18	N	4131	CN6	O11-C1	-2.53	1.35	1.44
15	N	4021	HEM	CBC-CAC	2.52	1.42	1.30
18	N	4131	CN6	OA-CB	2.49	1.50	1.43
18	C	4031	CN6	O11-C1	-2.49	1.35	1.44
17	C	4010	8PE	O32-C31	-2.49	1.15	1.22
17	N	4110	8PE	O32-C31	-2.44	1.15	1.22
15	C	4002	HEM	FE-NB	2.44	2.02	1.94
15	D	4003	HEM	FE-NA	2.43	2.03	1.95
16	N	4025	SMA	C20-C19	2.42	1.35	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	4003	HEM	FE-NB	2.40	2.02	1.94
15	C	4001	HEM	FE-NB	2.40	2.02	1.94
18	C	4031	CN6	OA-CB	2.37	1.50	1.43
20	O	4114	7PH	O22-C21	-2.29	1.15	1.22
15	N	4021	HEM	CMB-C2B	2.27	1.55	1.50
15	C	4001	HEM	CBB-CAB	2.25	1.41	1.30
22	L	4113	6PH	C1-C2	2.25	1.57	1.50
18	N	4131	CN6	O21-C21	2.23	1.40	1.34
15	C	4002	HEM	CAC-C3C	-2.22	1.41	1.47
15	N	4022	HEM	CAC-C3C	-2.22	1.41	1.47
18	N	4131	CN6	O41-C3'	-2.21	1.40	1.45
18	C	4031	CN6	O21-C21	2.16	1.40	1.34
14	A	4021	UMQ	O1'-C1'	2.12	1.43	1.40
22	L	4113	6PH	C3-C2	2.10	1.57	1.50
18	C	4031	CN6	O41-C3'	-2.09	1.40	1.45
20	D	4014	7PH	O22-C21	-2.09	1.16	1.22
15	W	4026	HEM	CMC-C2C	2.06	1.55	1.50
15	W	4026	HEM	CAB-C3B	2.06	1.52	1.47
15	C	4002	HEM	O2D-CGD	-2.06	1.24	1.30
15	O	4023	HEM	FE-NA	2.05	2.01	1.95
15	N	4021	HEM	FE-NB	2.05	2.01	1.94
17	C	4010	8PE	C3-C2	2.03	1.57	1.50
22	E	4013	6PH	C3-C2	2.03	1.57	1.50
15	W	4026	HEM	FE-NC	2.03	2.01	1.95
22	E	4013	6PH	C1-C2	2.02	1.57	1.50
22	E	4013	6PH	P-O11	-2.02	1.53	1.60

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	4121	UMQ	CA-O1'-C1'	-8.40	99.33	113.68
14	A	4021	UMQ	CA-O1'-C1'	-7.77	100.40	113.68
18	N	4131	CN6	C2'-O51-C51	-5.66	104.25	117.80
22	L	4113	6PH	C3-C2-C1	-4.45	101.42	111.78
18	C	4031	CN6	C2'-O51-C51	-4.32	107.45	117.80
22	E	4013	6PH	C3-C2-C1	-4.27	101.83	111.78
18	N	4131	CN6	C2-O21-C21	-4.08	108.04	117.80
18	C	4031	CN6	C2-O21-C21	-4.01	108.20	117.80
14	A	4021	UMQ	O1'-CA-CB	3.94	122.74	109.37
15	N	4021	HEM	CAD-C3D-C4D	3.89	131.47	124.70
20	O	4114	7PH	O12-P-O11	3.85	116.70	106.67
22	E	4013	6PH	O11-P-O12	3.81	116.73	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	4131	CN6	C3'-C2'-C1'	-3.80	102.93	111.78
22	L	4113	6PH	O11-P-O12	3.76	116.61	106.44
19	C	4111	9PE	C2-O21-C21	-3.69	108.95	117.80
14	L	4121	UMQ	O1'-CA-CB	3.68	121.84	109.37
18	C	4031	CN6	C3-C2-C1	-3.67	103.22	111.78
20	D	4014	7PH	C38-C37-C36	-3.63	96.01	114.37
20	D	4014	7PH	O12-P-O11	3.61	116.08	106.67
18	N	4131	CN6	C3-C2-C1	-3.56	103.48	111.78
15	D	4003	HEM	CBB-CAB-C3B	-3.55	109.79	127.53
17	N	4110	8PE	C2-O21-C21	-3.51	109.39	117.80
15	O	4023	HEM	CBB-CAB-C3B	-3.50	110.04	127.53
15	W	4026	HEM	CAC-C3C-C4C	-3.46	116.55	124.82
20	O	4114	7PH	C38-C37-C36	-3.45	96.92	114.37
17	N	4110	8PE	C3-C2-C1	3.45	119.83	111.78
18	N	4131	CN6	P-O13-CC	3.37	140.67	121.35
15	N	4021	HEM	CAD-C3D-C2D	-3.32	121.65	127.87
15	D	4003	HEM	CBC-CAC-C3C	-3.24	111.34	127.53
22	L	4113	6PH	O13-P-O11	3.20	115.00	106.67
17	C	4010	8PE	C2-O21-C21	-3.18	110.20	117.80
18	C	4031	CN6	P-O13-CC	3.16	139.46	121.35
19	N	4011	9PE	C2-O21-C21	-3.14	110.29	117.80
15	D	4003	HEM	CAD-C3D-C4D	3.08	130.07	124.70
15	W	4026	HEM	CBB-CAB-C3B	-3.07	112.19	127.53
15	W	4026	HEM	CBC-CAC-C3C	-3.00	112.53	127.53
22	E	4013	6PH	O13-P-O11	2.98	114.44	106.67
18	C	4031	CN6	P-O11-C1	-2.97	104.34	121.35
20	D	4014	7PH	C3-C2-C1	-2.95	104.90	111.78
15	D	4003	HEM	CMD-C2D-C1D	2.89	129.55	125.03
15	C	4001	HEM	CAB-C3B-C2B	-2.88	119.07	128.43
20	O	4114	7PH	O13-P-O11	2.83	114.06	106.67
22	L	4113	6PH	O14-P-O11	-2.77	99.44	106.67
18	N	4131	CN6	P-O11-C1	-2.77	105.48	121.35
18	N	4131	CN6	O3'-P'-O4'	2.76	119.86	108.94
20	O	4114	7PH	O31-C3-C2	-2.72	100.55	108.40
18	C	4031	CN6	O3'-P'-O4'	2.68	119.57	108.94
15	O	4023	HEM	CAD-C3D-C4D	2.68	129.36	124.70
15	O	4023	HEM	CAC-C3C-C4C	-2.66	118.47	124.82
22	E	4013	6PH	O14-P-O11	-2.64	99.78	106.67
15	C	4001	HEM	CMC-C2C-C1C	2.63	129.37	124.73
15	O	4023	HEM	CAA-C2A-C1A	2.61	130.04	124.94
18	C	4031	CN6	C3'-C2'-C1'	-2.59	105.74	111.78
15	W	4026	HEM	CAC-C3C-C2C	2.58	136.81	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	4014	7PH	O13-P-O11	2.57	113.37	106.67
15	D	4003	HEM	CAD-C3D-C2D	-2.56	123.06	127.87
15	O	4023	HEM	CBC-CAC-C3C	-2.55	114.77	127.53
16	C	4005	SMA	C4A-C4-C3	-2.55	115.02	118.78
20	O	4114	7PH	O11-P-O14	-2.53	99.59	106.44
20	O	4114	7PH	C3-C2-C1	-2.53	105.89	111.78
14	A	4021	UMQ	C3'-C4'-C5'	-2.49	105.41	110.93
14	L	4121	UMQ	C3'-C4'-C5'	-2.47	105.46	110.93
17	N	4110	8PE	O31-C3-C2	-2.46	101.31	108.40
20	O	4114	7PH	O31-C31-C32	-2.44	104.39	111.83
16	C	4005	SMA	O8-C8-C7	2.41	124.38	119.21
14	A	4021	UMQ	CD-CC-CB	-2.40	102.25	114.37
18	N	4131	CN6	P'-O3'-CA	2.39	135.04	121.35
18	N	4131	CN6	OA-CB-CA	2.35	117.82	109.70
14	L	4121	UMQ	CD-CC-CB	-2.33	102.58	114.37
20	D	4014	7PH	O11-P-O14	-2.32	100.18	106.44
16	N	4025	SMA	C4A-C4-C3	-2.31	115.37	118.78
18	C	4031	CN6	P'-O3'-CA	2.31	134.56	121.35
15	N	4022	HEM	CMB-C2B-C1B	-2.30	121.44	125.03
20	D	4014	7PH	O31-C31-C32	-2.27	104.92	111.83
20	D	4014	7PH	O31-C31-O32	2.21	129.15	123.63
20	O	4114	7PH	O31-C31-O32	2.19	129.10	123.63
20	D	4014	7PH	O12-P-O14	-2.17	102.38	110.83
14	A	4021	UMQ	O1-C1-O5	-2.14	105.05	110.69
18	C	4031	CN6	O2'-P'-O4'	-2.14	102.47	112.44
15	N	4021	HEM	CBA-CAA-C2A	-2.14	106.61	112.53
15	O	4023	HEM	CAD-C3D-C2D	-2.14	123.86	127.87
14	L	4121	UMQ	O1'-C1'-C2'	2.13	111.52	108.27
20	D	4014	7PH	O31-C3-C2	-2.10	102.34	108.40
20	O	4114	7PH	O12-P-O14	-2.10	102.67	110.83
18	N	4131	CN6	O14-P-O12	-2.07	102.81	112.44
15	C	4001	HEM	CAB-C3B-C4B	2.07	133.53	124.39
18	N	4131	CN6	O2'-P'-O4'	-2.06	102.84	112.44
18	N	4131	CN6	O14-P-O13	2.05	116.88	107.57
15	W	4026	HEM	CBD-CAD-C3D	-2.05	106.86	112.53
18	C	4031	CN6	O14-P-O12	-2.02	103.03	112.44
14	A	4021	UMQ	C1-O5-C5	-2.02	109.78	113.72
14	A	4021	UMQ	CC-CB-CA	2.01	122.22	113.47

There are no chirality outliers.

All (254) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	O	4023	HEM	C2C-C3C-CAC-CBC
18	C	4031	CN6	CC-O13-P-O11
18	C	4031	CN6	CC-O13-P-O12
18	C	4031	CN6	CC-O13-P-O14
18	C	4031	CN6	O11-C1-C2-O21
18	C	4031	CN6	O32-C31-O31-C3
18	C	4031	CN6	C22-C21-O21-C2
18	C	4031	CN6	CA-O3'-P'-O1'
18	C	4031	CN6	CA-O3'-P'-O2'
18	C	4031	CN6	CA-O3'-P'-O4'
18	C	4031	CN6	O1'-C1'-C2'-O51
18	C	4031	CN6	O52-C51-O51-C2'
18	C	4031	CN6	C52-C51-O51-C2'
18	C	4031	CN6	O3'-CA-CB-CC
18	N	4131	CN6	C1-O11-P-O14
18	N	4131	CN6	CC-O13-P-O11
18	N	4131	CN6	CC-O13-P-O12
18	N	4131	CN6	CC-O13-P-O14
18	N	4131	CN6	O11-C1-C2-O21
18	N	4131	CN6	C22-C21-O21-C2
18	N	4131	CN6	CA-O3'-P'-O1'
18	N	4131	CN6	CA-O3'-P'-O2'
18	N	4131	CN6	CA-O3'-P'-O4'
18	N	4131	CN6	O1'-C1'-C2'-O51
18	N	4131	CN6	C52-C51-O51-C2'
19	C	4111	9PE	C1-O11-P-O12
19	C	4111	9PE	C1-O11-P-O13
19	C	4111	9PE	C1-O11-P-O14
19	C	4111	9PE	C11-O13-P-O11
19	C	4111	9PE	C11-O13-P-O12
19	N	4011	9PE	C1-O11-P-O12
19	N	4011	9PE	C1-O11-P-O13
19	N	4011	9PE	C1-O11-P-O14
19	N	4011	9PE	C11-O13-P-O11
19	N	4011	9PE	C11-O13-P-O12
19	N	4011	9PE	O13-C11-C12-N
18	N	4131	CN6	O32-C31-O31-C3
18	C	4031	CN6	O22-C21-O21-C2
18	N	4131	CN6	O22-C21-O21-C2
18	N	4131	CN6	O52-C51-O51-C2'
18	C	4031	CN6	C32-C31-O31-C3
18	N	4131	CN6	C32-C31-O31-C3
18	C	4031	CN6	O3'-CA-CB-OA

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Mol	Chain	Res	Type	Atoms
14	A	4021	UMQ	O1'-CA-CB-CC
14	L	4121	UMQ	O1'-CA-CB-CC
20	O	4114	7PH	C21-C22-C23-C24
22	L	4113	6PH	C2B-C2C-C2D-C2E
17	N	4110	8PE	C21-C22-C23-C24
20	O	4114	7PH	C31-C32-C33-C34
18	C	4031	CN6	C41-C42-C43-C44
20	D	4014	7PH	C31-C32-C33-C34
18	N	4131	CN6	O3'-CA-CB-OA
19	N	4011	9PE	C31-C32-C33-C34
18	N	4131	CN6	O3'-CA-CB-CC
19	N	4011	9PE	C2E-C2F-C2G-C2H
16	N	4025	SMA	C9-C10-C11-C22
17	C	4010	8PE	C37-C38-C39-C3A
22	L	4113	6PH	C22-C21-O21-C2
17	N	4110	8PE	C37-C38-C39-C3A
20	D	4014	7PH	C27-C28-C29-C2A
22	L	4113	6PH	C37-C38-C39-C3A
19	N	4011	9PE	C28-C29-C2A-C2B
17	C	4010	8PE	C38-C39-C3A-C3B
19	C	4111	9PE	C2E-C2F-C2G-C2H
19	N	4011	9PE	C32-C33-C34-C35
22	L	4113	6PH	O22-C21-O21-C2
17	N	4110	8PE	O11-C1-C2-C3
17	C	4010	8PE	C24-C25-C26-C27
20	O	4114	7PH	C2A-C2B-C2C-C2D
17	C	4010	8PE	C33-C34-C35-C36
18	N	4131	CN6	C46-C47-C48-C49
19	C	4111	9PE	C26-C27-C28-C29
20	D	4014	7PH	C32-C33-C34-C35
22	E	4013	6PH	C35-C36-C37-C38
22	E	4013	6PH	C29-C2A-C2B-C2C
17	N	4110	8PE	C3B-C3C-C3D-C3E
22	E	4013	6PH	C27-C28-C29-C2A
22	L	4113	6PH	C29-C2A-C2B-C2C
14	L	4121	UMQ	CF-CG-CH-CI
17	N	4110	8PE	C33-C34-C35-C36
17	C	4010	8PE	C26-C27-C28-C29
22	E	4013	6PH	C22-C21-O21-C2
17	C	4010	8PE	C34-C35-C36-C37
22	L	4113	6PH	C38-C39-C3A-C3B
17	N	4110	8PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
17	N	4110	8PE	C39-C3A-C3B-C3C
19	N	4011	9PE	C23-C24-C25-C26
18	C	4031	CN6	C42-C43-C44-C45
17	N	4110	8PE	C3E-C3F-C3G-C3H
22	L	4113	6PH	C36-C37-C38-C39
14	A	4021	UMQ	CF-CG-CH-CI
17	N	4110	8PE	C28-C29-C2A-C2B
18	C	4031	CN6	C43-C44-C45-C46
22	E	4013	6PH	C36-C37-C38-C39
19	C	4111	9PE	C2D-C2E-C2F-C2G
20	D	4014	7PH	C22-C21-O21-C2
20	D	4014	7PH	O22-C21-O21-C2
15	D	4003	HEM	C2C-C3C-CAC-CBC
17	C	4010	8PE	C3A-C3B-C3C-C3D
17	N	4110	8PE	C29-C2A-C2B-C2C
20	O	4114	7PH	C32-C33-C34-C35
17	C	4010	8PE	C39-C3A-C3B-C3C
20	D	4014	7PH	C22-C23-C24-C25
15	O	4023	HEM	C4C-C3C-CAC-CBC
17	N	4110	8PE	C2A-C2B-C2C-C2D
19	N	4011	9PE	C2B-C2C-C2D-C2E
20	D	4014	7PH	C34-C35-C36-C37
22	L	4113	6PH	C27-C28-C29-C2A
20	O	4114	7PH	C22-C23-C24-C25
22	L	4113	6PH	C34-C35-C36-C37
17	C	4010	8PE	C2A-C2B-C2C-C2D
19	N	4011	9PE	C2C-C2D-C2E-C2F
20	D	4014	7PH	C37-C38-C39-C3A
17	C	4010	8PE	O11-C1-C2-C3
18	C	4031	CN6	O11-C1-C2-C3
18	C	4031	CN6	O1'-C1'-C2'-C3'
18	N	4131	CN6	O11-C1-C2-C3
18	N	4131	CN6	O1'-C1'-C2'-C3'
19	N	4011	9PE	O11-C1-C2-C3
22	E	4013	6PH	O11-C1-C2-C3
18	C	4031	CN6	C48-C49-C4A-C4B
22	L	4113	6PH	C35-C36-C37-C38
17	C	4010	8PE	C36-C37-C38-C39
19	N	4011	9PE	C26-C27-C28-C29
15	D	4003	HEM	C4D-C3D-CAD-CBD
15	O	4023	HEM	C4D-C3D-CAD-CBD
22	E	4013	6PH	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
20	O	4114	7PH	C37-C38-C39-C3A
19	N	4011	9PE	C22-C23-C24-C25
18	N	4131	CN6	C42-C41-O41-C3'
20	D	4014	7PH	C26-C27-C28-C29
17	N	4110	8PE	C36-C37-C38-C39
20	O	4114	7PH	C27-C28-C29-C2A
18	C	4031	CN6	C47-C48-C49-C4A
22	E	4013	6PH	C28-C29-C2A-C2B
22	L	4113	6PH	C25-C26-C27-C28
20	O	4114	7PH	C23-C24-C25-C26
22	E	4013	6PH	C24-C25-C26-C27
22	L	4113	6PH	C3A-C3B-C3C-C3D
19	C	4111	9PE	O11-C1-C2-C3
22	L	4113	6PH	O11-C1-C2-C3
17	N	4110	8PE	C2B-C2C-C2D-C2E
18	N	4131	CN6	C41-C42-C43-C44
18	N	4131	CN6	O42-C41-O41-C3'
19	C	4111	9PE	C24-C25-C26-C27
20	D	4014	7PH	C28-C29-C2A-C2B
17	C	4010	8PE	C29-C2A-C2B-C2C
14	L	4121	UMQ	CI-CJ-CK-CL
17	C	4010	8PE	O11-C1-C2-O21
17	N	4110	8PE	O11-C1-C2-O21
19	C	4111	9PE	O11-C1-C2-O21
22	L	4113	6PH	C39-C3A-C3B-C3C
17	C	4010	8PE	C3E-C3F-C3G-C3H
14	A	4021	UMQ	CI-CJ-CK-CL
16	C	4005	SMA	C9-C10-C11-C22
19	C	4111	9PE	C23-C24-C25-C26
20	D	4014	7PH	C2B-C2C-C2D-C2E
15	D	4003	HEM	C2B-C3B-CAB-CBB
15	N	4021	HEM	C2C-C3C-CAC-CBC
15	O	4023	HEM	C2B-C3B-CAB-CBB
15	W	4026	HEM	C2B-C3B-CAB-CBB
15	W	4026	HEM	C2C-C3C-CAC-CBC
16	C	4005	SMA	C15-C14-O14-C25
19	N	4011	9PE	C2D-C2E-C2F-C2G
19	C	4111	9PE	C21-C22-C23-C24
19	N	4011	9PE	O11-C1-C2-O21
22	L	4113	6PH	C28-C29-C2A-C2B
15	W	4026	HEM	C4B-C3B-CAB-CBB
15	D	4003	HEM	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
17	N	4110	8PE	C3A-C3B-C3C-C3D
19	N	4011	9PE	C12-C11-O13-P
19	C	4111	9PE	C2A-C2B-C2C-C2D
19	N	4011	9PE	C2A-C2B-C2C-C2D
20	D	4014	7PH	C23-C24-C25-C26
18	N	4131	CN6	O31-C31-C32-C33
22	L	4113	6PH	C33-C34-C35-C36
17	C	4010	8PE	C23-C24-C25-C26
18	C	4031	CN6	CB-CC-O13-P
22	E	4013	6PH	O11-C1-C2-O21
22	L	4113	6PH	O11-C1-C2-O21
18	C	4031	CN6	O32-C31-C32-C33
17	C	4010	8PE	C32-C33-C34-C35
17	C	4010	8PE	C28-C29-C2A-C2B
17	C	4010	8PE	O13-C11-C12-N
19	C	4111	9PE	O13-C11-C12-N
18	C	4031	CN6	O31-C31-C32-C33
17	N	4110	8PE	C3D-C3E-C3F-C3G
22	E	4013	6PH	C37-C38-C39-C3A
19	C	4111	9PE	C2B-C2C-C2D-C2E
19	N	4011	9PE	C29-C2A-C2B-C2C
15	O	4023	HEM	C2D-C3D-CAD-CBD
18	N	4131	CN6	O32-C31-C32-C33
22	L	4113	6PH	C24-C25-C26-C27
17	N	4110	8PE	C31-C32-C33-C34
22	E	4013	6PH	C2B-C2C-C2D-C2E
17	N	4110	8PE	C24-C25-C26-C27
15	D	4003	HEM	C4B-C3B-CAB-CBB
15	D	4003	HEM	C4C-C3C-CAC-CBC
15	N	4021	HEM	C4C-C3C-CAC-CBC
15	O	4023	HEM	C4B-C3B-CAB-CBB
15	W	4026	HEM	C4C-C3C-CAC-CBC
15	C	4001	HEM	CAD-CBD-CGD-O1D
18	N	4131	CN6	C51-C52-C53-C54
19	C	4111	9PE	C2C-C2D-C2E-C2F
15	N	4022	HEM	CAA-CBA-CGA-O1A
15	N	4022	HEM	CAA-CBA-CGA-O2A
22	L	4113	6PH	C32-C33-C34-C35
19	C	4111	9PE	O31-C31-C32-C33
15	C	4001	HEM	CAA-CBA-CGA-O2A
15	N	4021	HEM	CAD-CBD-CGD-O2D
20	O	4114	7PH	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
15	C	4001	HEM	CAD-CBD-CGD-O2D
15	C	4002	HEM	CAA-CBA-CGA-O1A
15	C	4001	HEM	CAA-CBA-CGA-O1A
15	N	4021	HEM	CAD-CBD-CGD-O1D
18	N	4131	CN6	CB-CC-O13-P
15	N	4022	HEM	CAD-CBD-CGD-O2D
15	O	4023	HEM	CAD-CBD-CGD-O2D
15	D	4003	HEM	CAD-CBD-CGD-O2D
15	C	4002	HEM	CAA-CBA-CGA-O2A
15	O	4023	HEM	CAA-CBA-CGA-O2A
14	A	4021	UMQ	CG-CH-CI-CJ
15	O	4023	HEM	CAA-CBA-CGA-O1A
20	D	4014	7PH	C25-C26-C27-C28
22	E	4013	6PH	C2C-C2D-C2E-C2F
15	D	4003	HEM	CAD-CBD-CGD-O1D
15	D	4003	HEM	CAA-CBA-CGA-O2A
15	N	4022	HEM	CAD-CBD-CGD-O1D
17	C	4010	8PE	C31-C32-C33-C34
15	O	4023	HEM	CAD-CBD-CGD-O1D
22	E	4013	6PH	C33-C34-C35-C36
22	E	4013	6PH	O31-C31-C32-C33
15	D	4003	HEM	CAA-CBA-CGA-O1A
20	O	4114	7PH	C25-C26-C27-C28
15	N	4021	HEM	CAA-CBA-CGA-O1A
15	N	4021	HEM	CAA-CBA-CGA-O2A
15	C	4002	HEM	CAD-CBD-CGD-O2D
19	C	4111	9PE	C25-C26-C27-C28
17	C	4010	8PE	O21-C21-C22-C23
20	O	4114	7PH	C28-C29-C2A-C2B
17	C	4010	8PE	C21-C22-C23-C24
15	C	4002	HEM	CAD-CBD-CGD-O1D
17	C	4010	8PE	C2B-C2C-C2D-C2E
22	E	4013	6PH	C25-C26-C27-C28
20	O	4114	7PH	C35-C36-C37-C38
17	C	4010	8PE	O22-C21-C22-C23
15	W	4026	HEM	CAA-CBA-CGA-O2A
22	E	4013	6PH	O32-C31-C32-C33
20	D	4014	7PH	C2A-C2B-C2C-C2D
22	L	4113	6PH	C22-C23-C24-C25
15	N	4022	HEM	C2C-C3C-CAC-CBC
14	L	4121	UMQ	CD-CF-CG-CH
15	W	4026	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	N	4011	9PE	O31-C31-C32-C33

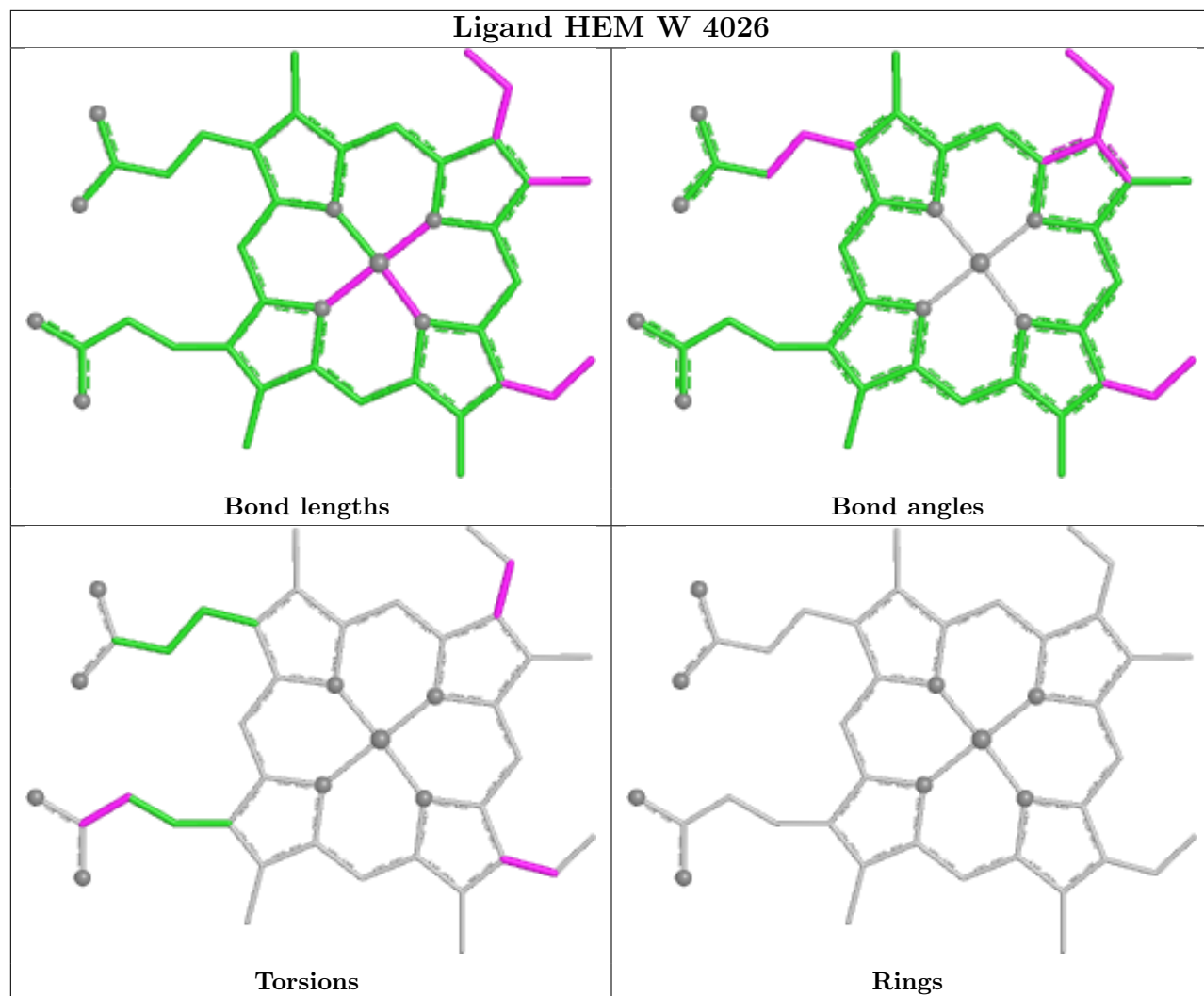
There are no ring outliers.

17 monomers are involved in 40 short contacts:

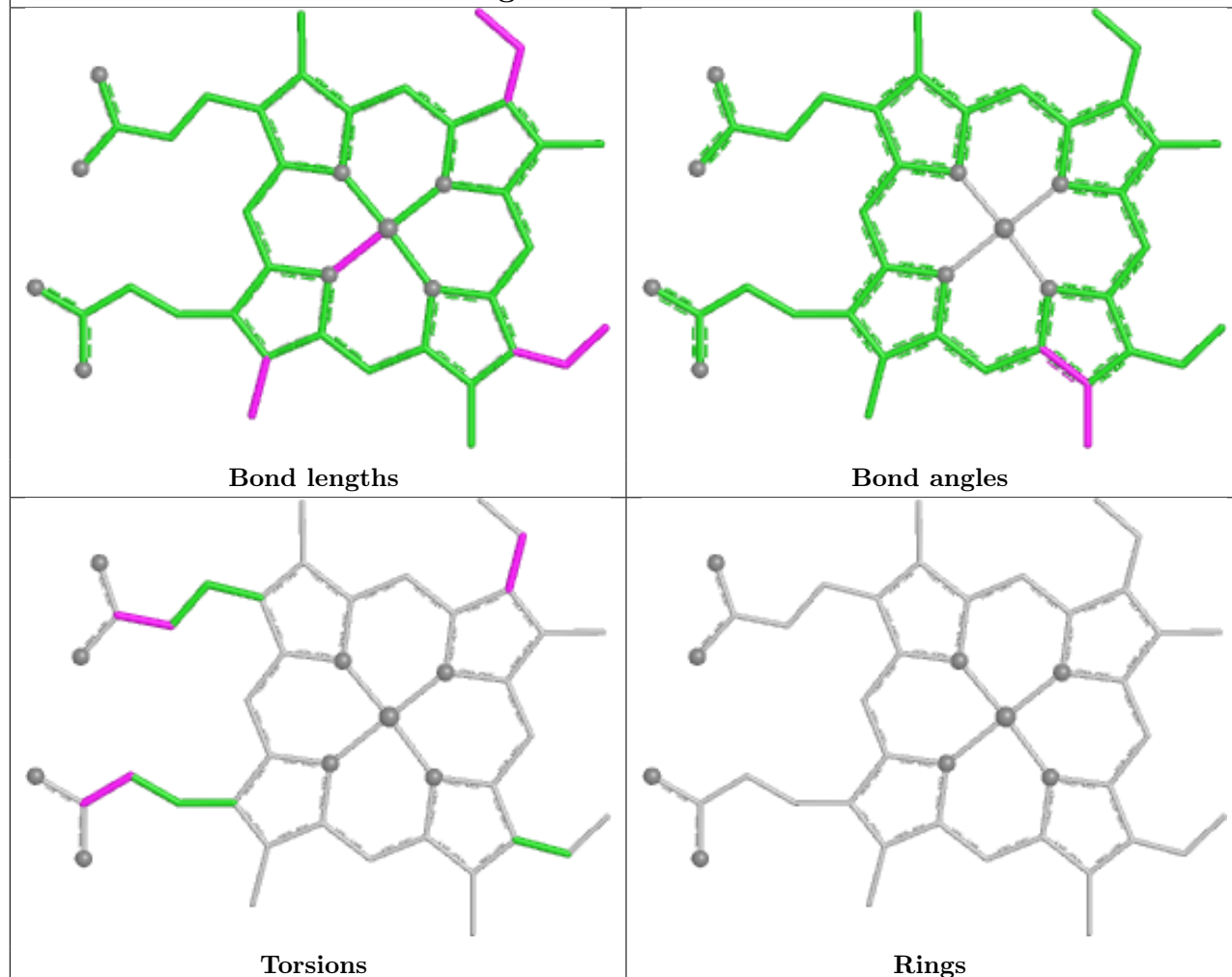
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	W	4026	HEM	2	0
15	N	4022	HEM	1	0
20	O	4114	7PH	2	0
20	D	4014	7PH	3	0
14	L	4121	UMQ	2	0
17	N	4110	8PE	2	0
15	O	4023	HEM	1	0
21	P	4024	FES	1	0
15	C	4002	HEM	1	0
22	E	4013	6PH	2	0
18	N	4131	CN6	5	0
18	C	4031	CN6	9	0
17	C	4010	8PE	2	0
16	C	4005	SMA	1	0
14	A	4021	UMQ	4	0
15	C	4001	HEM	2	0
16	N	4025	SMA	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.

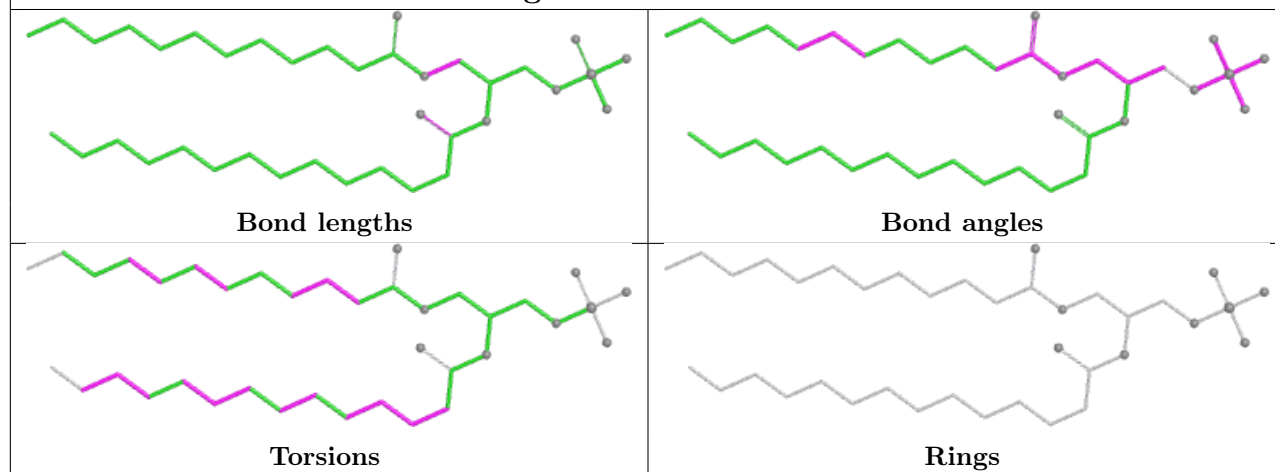
Ligand HEM W 4026

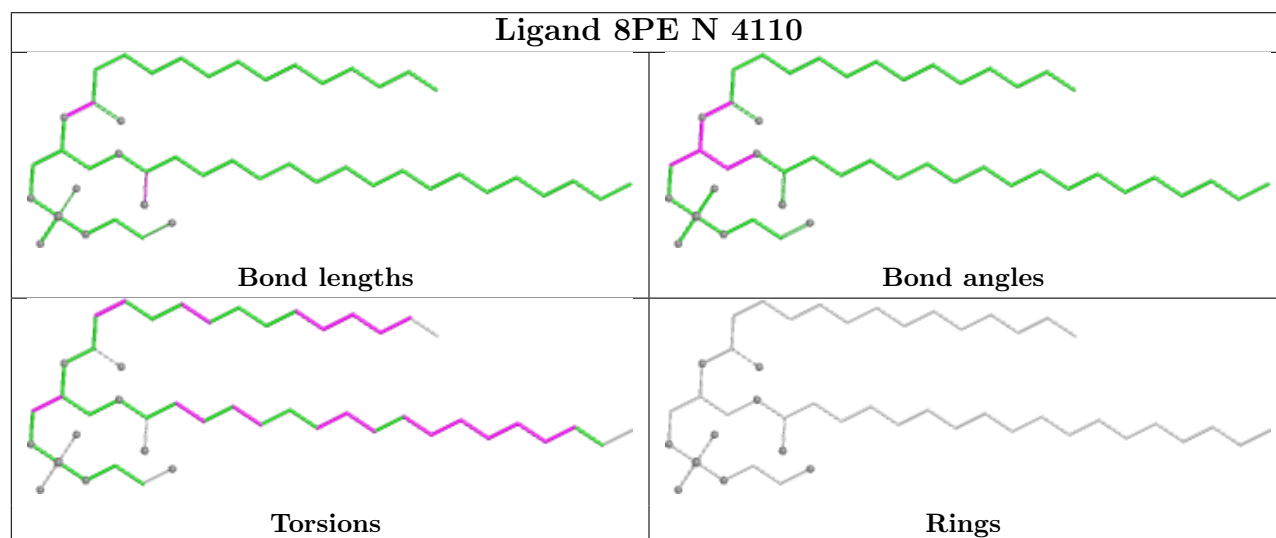
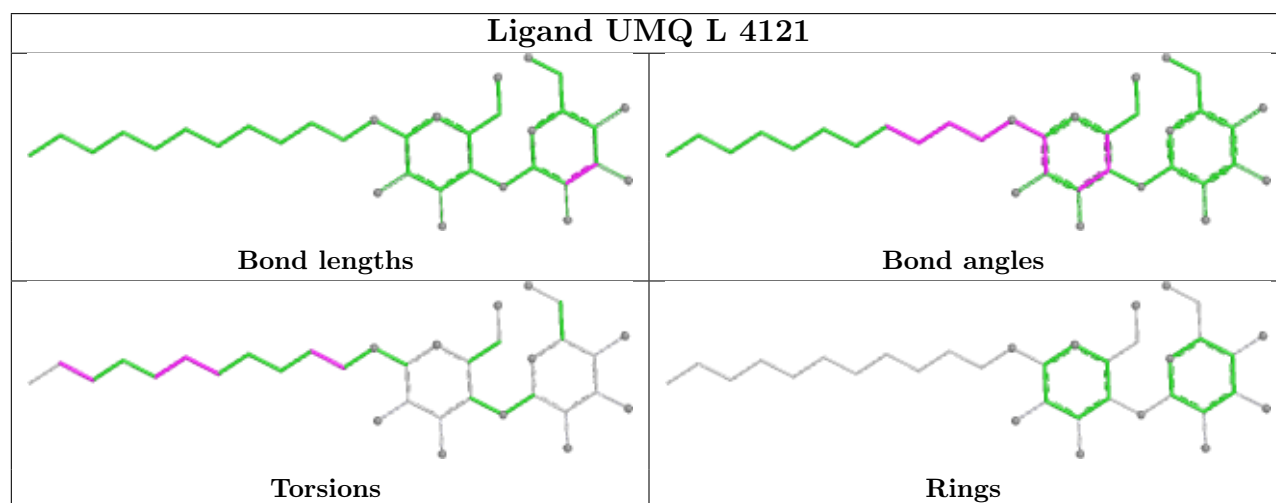
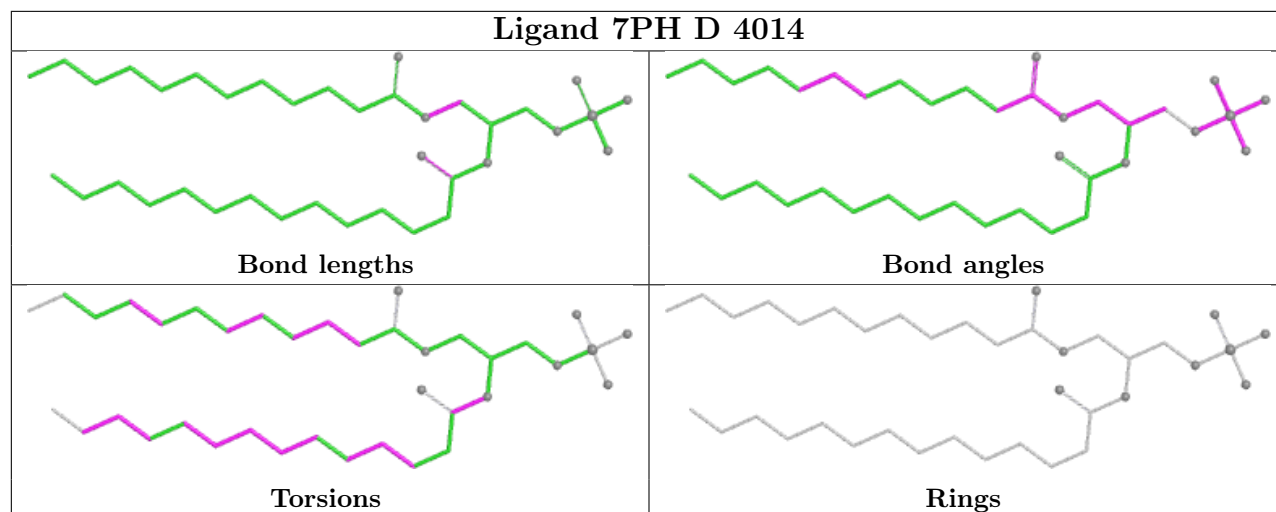


Ligand HEM N 4022

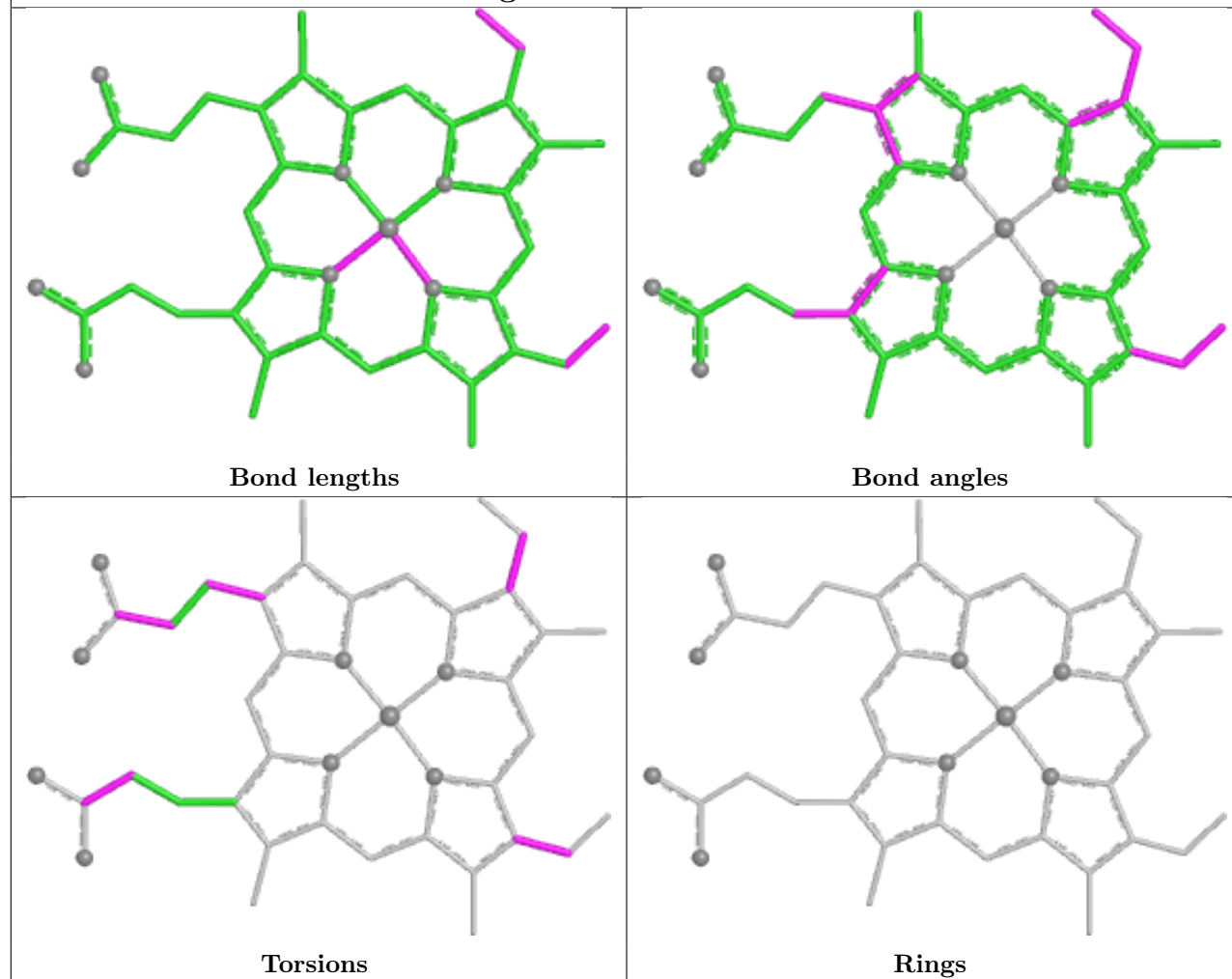


Ligand 7PH O 4114

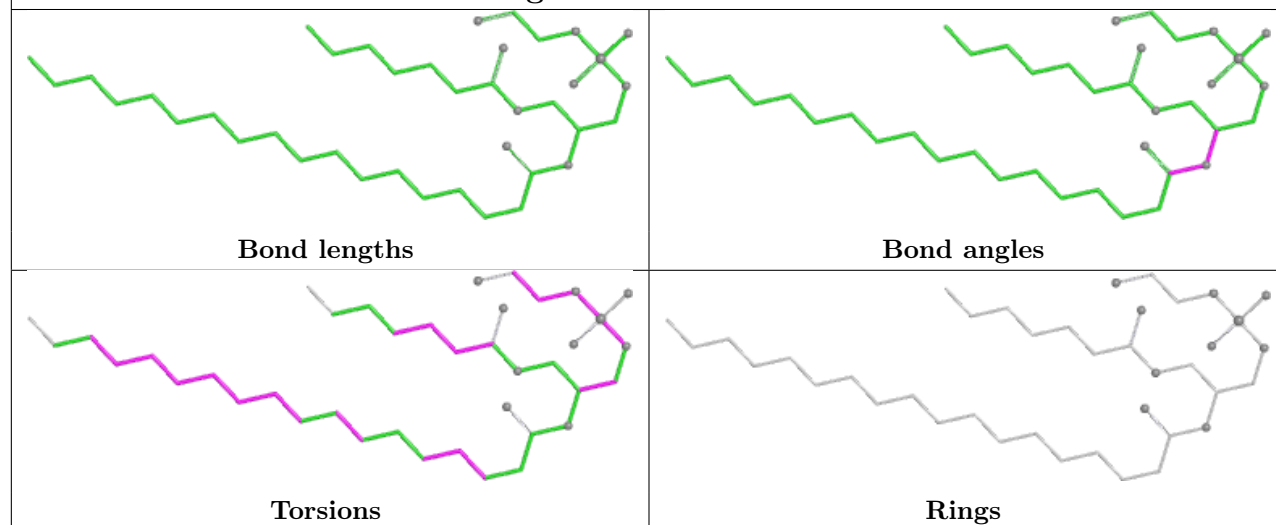


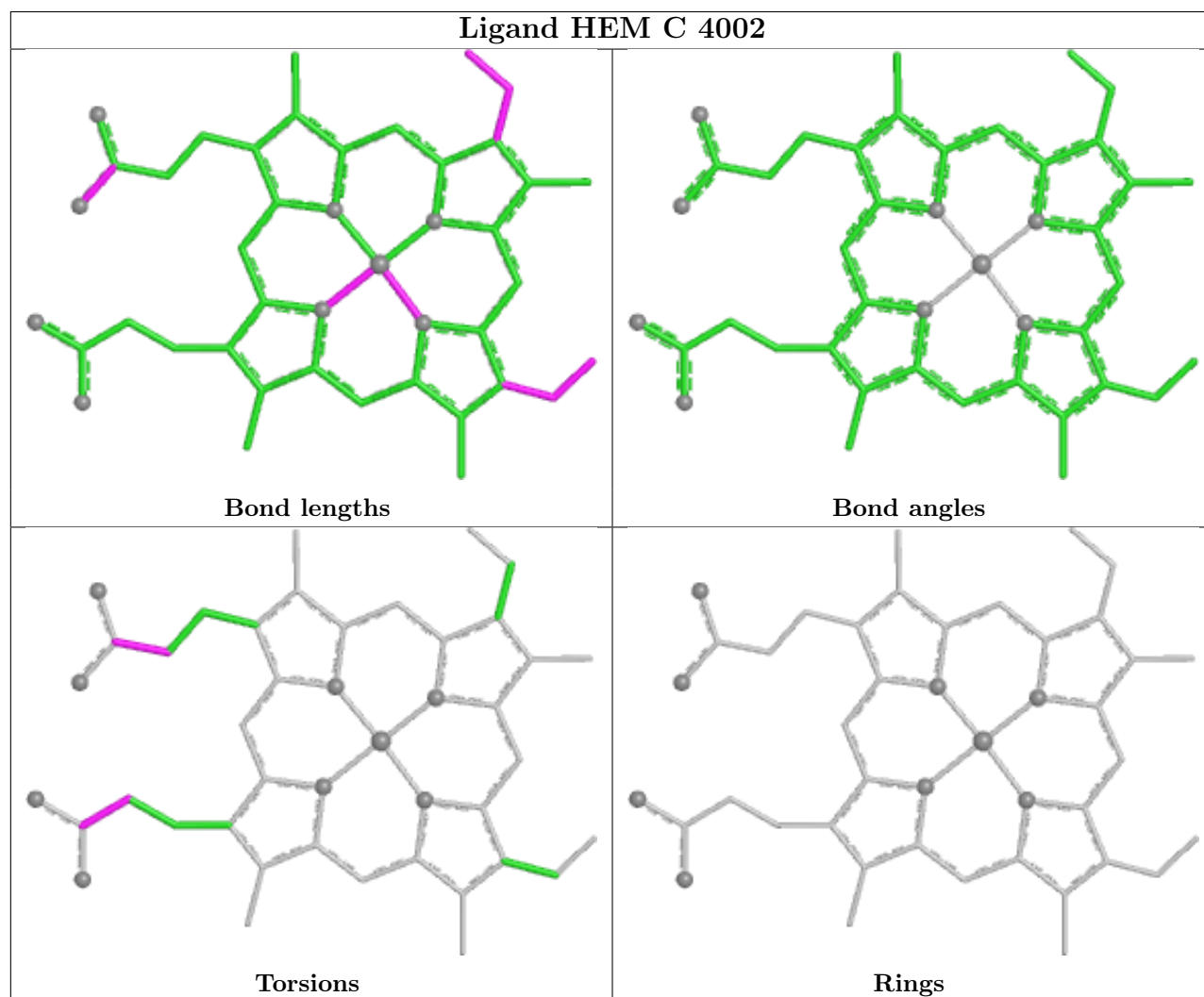
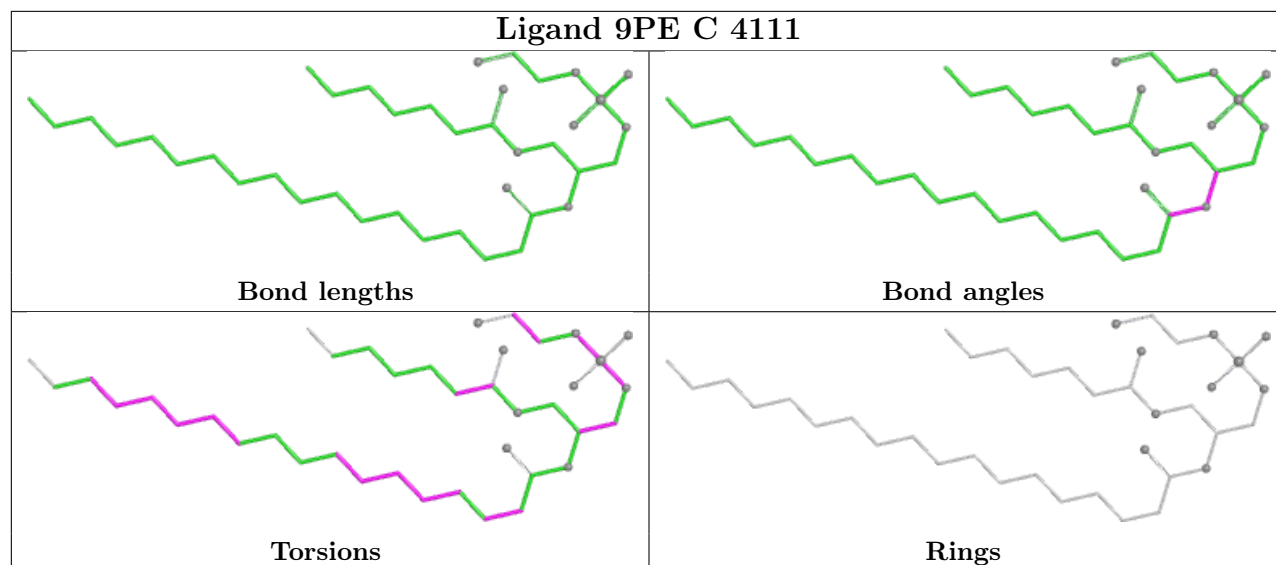


Ligand HEM O 4023

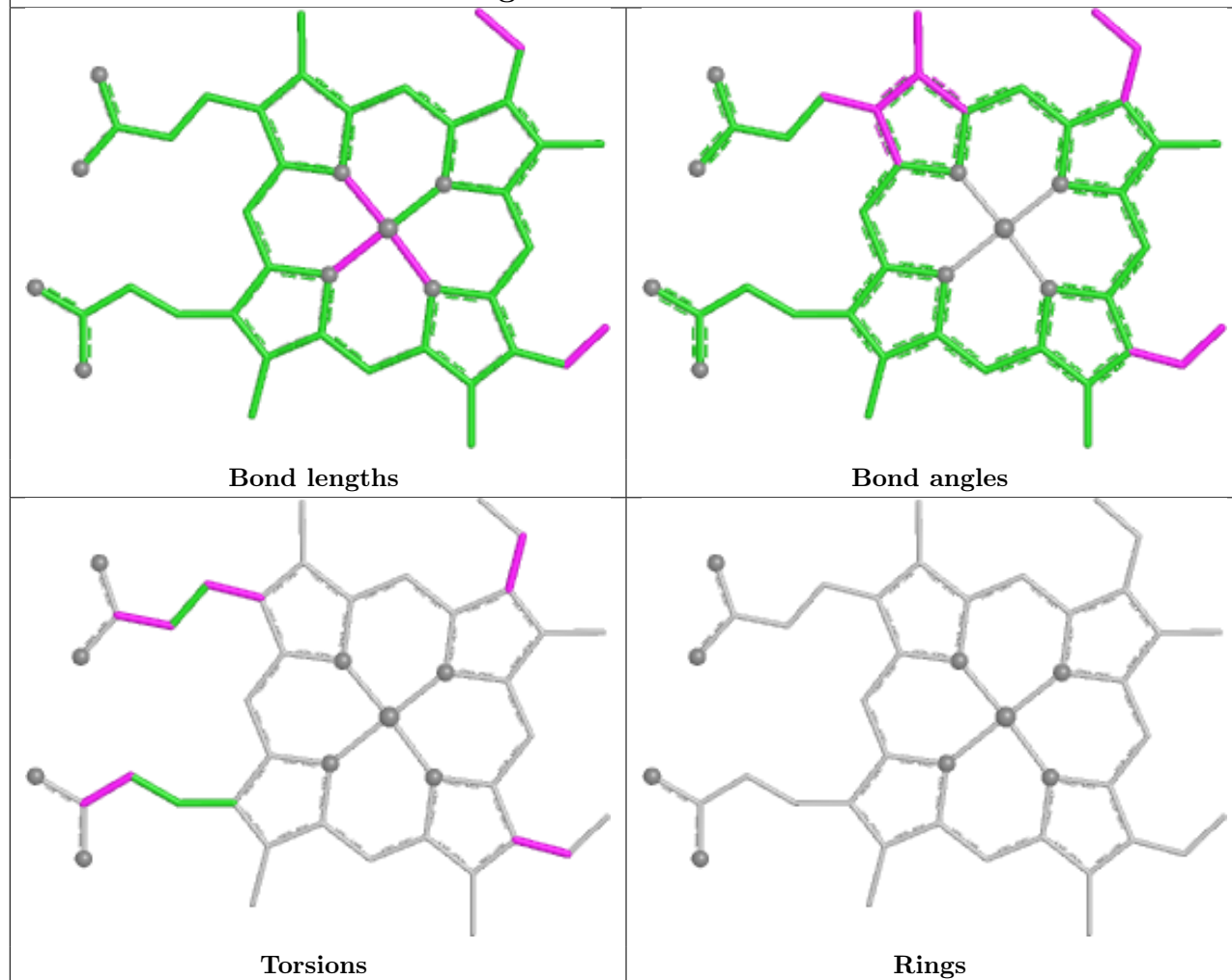


Ligand 9PE N 4011

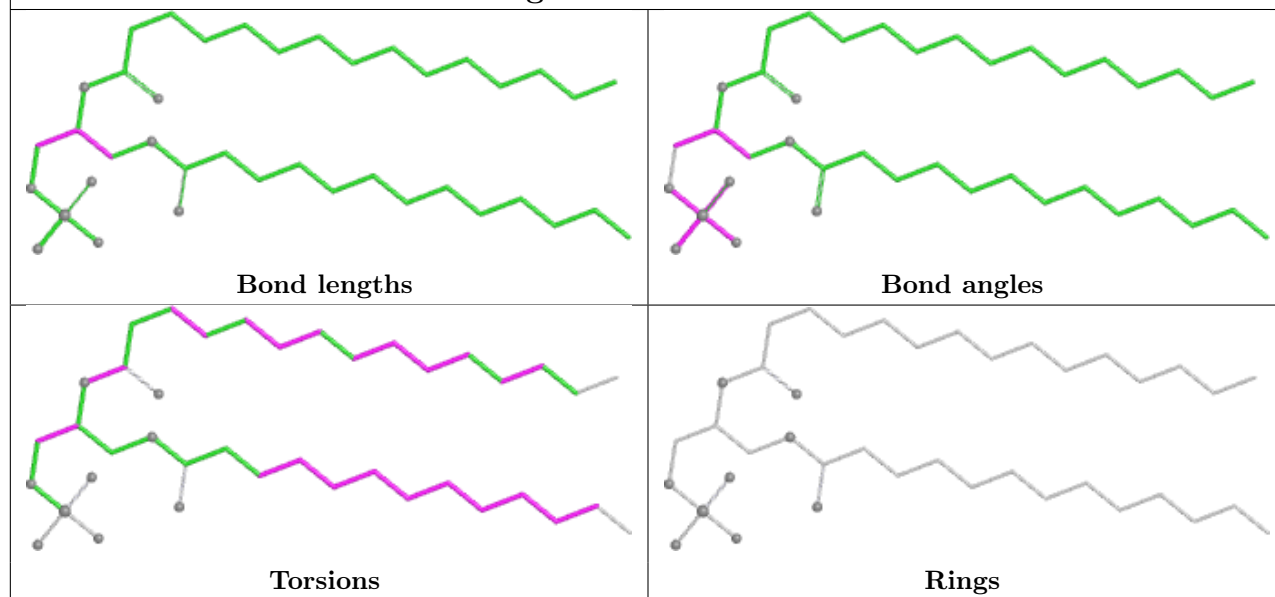


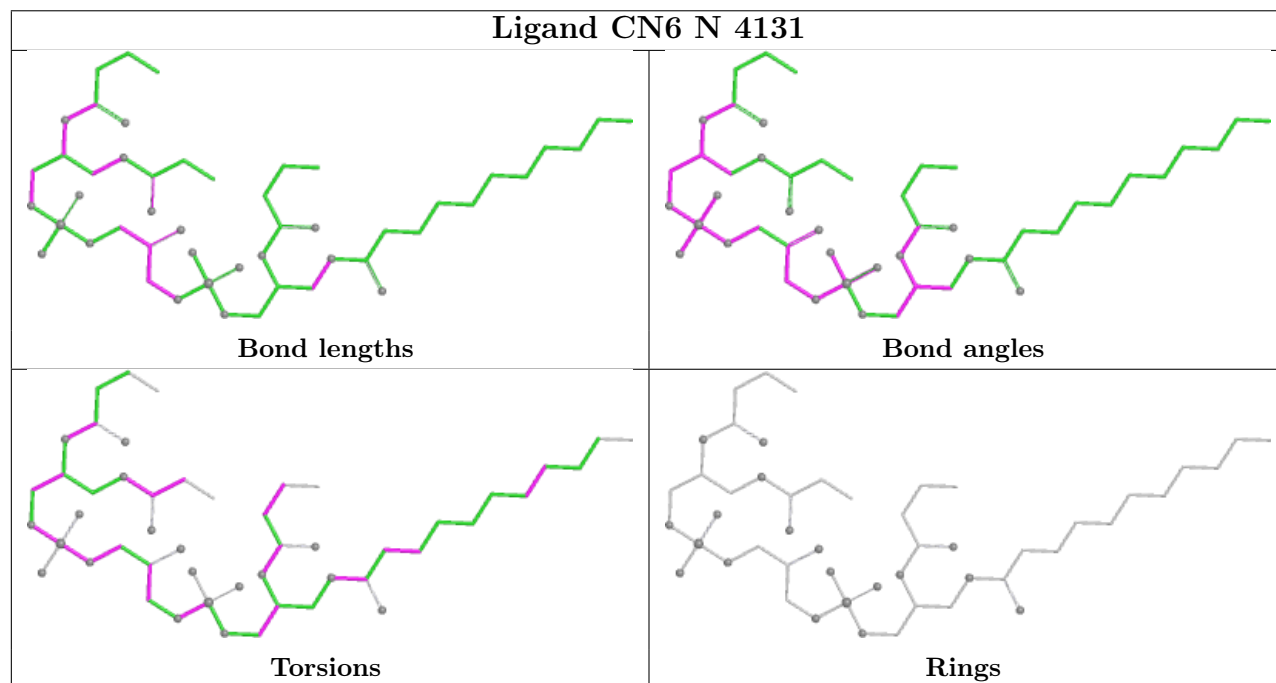
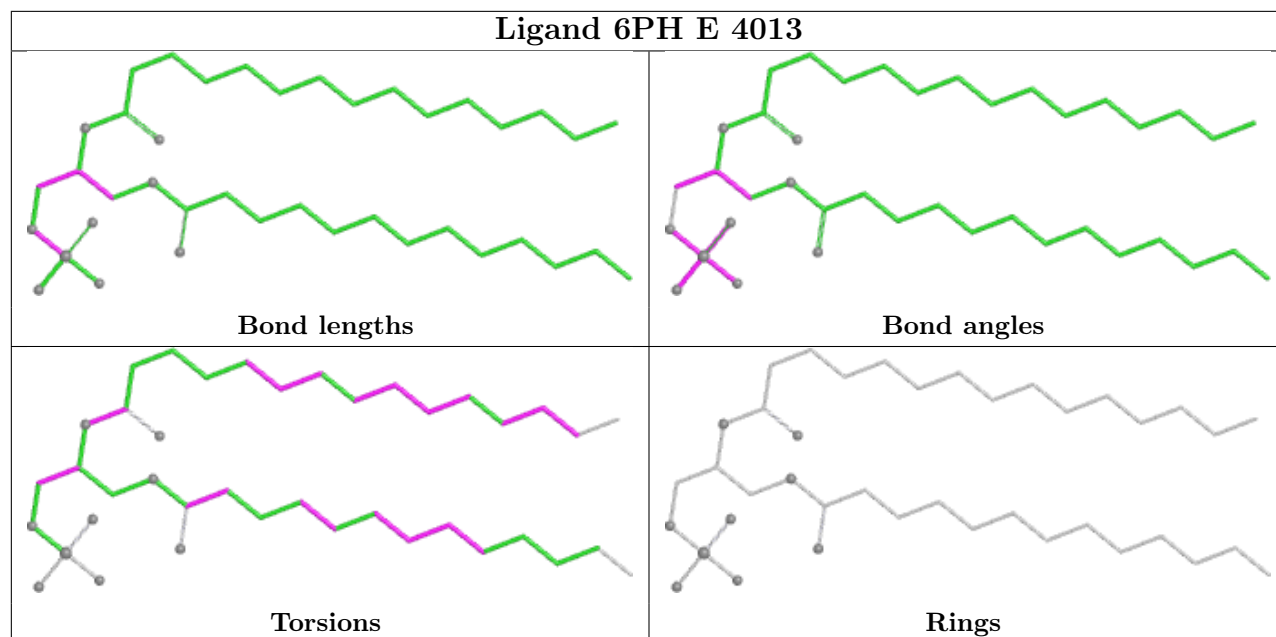


Ligand HEM D 4003

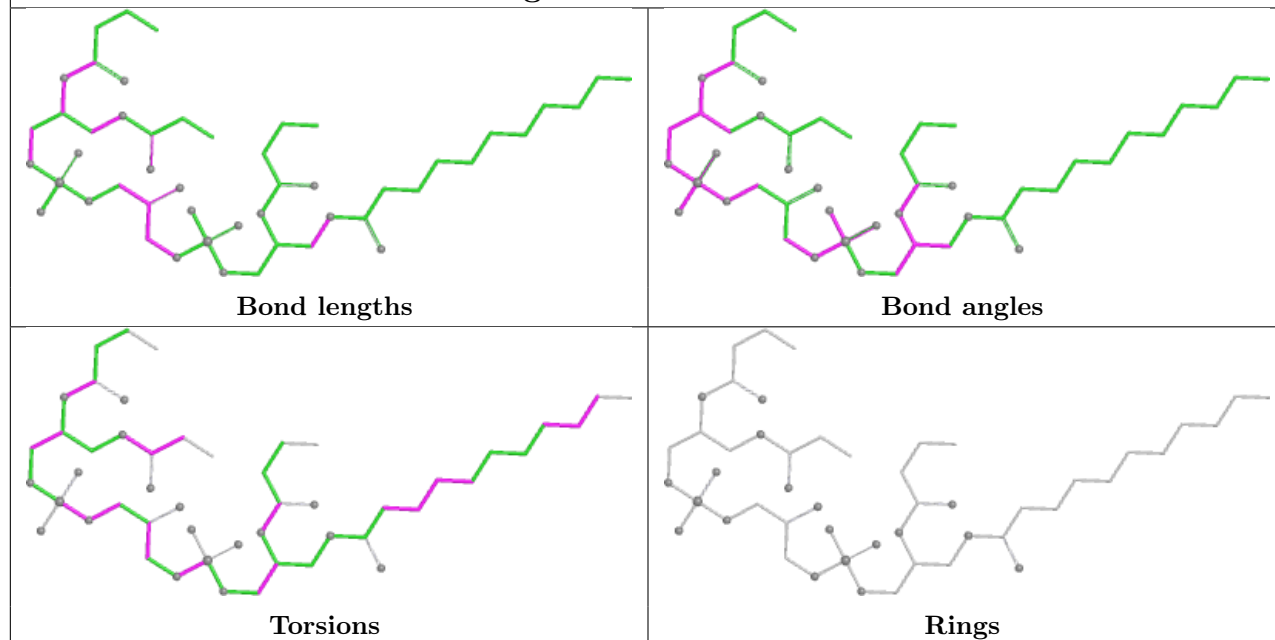


Ligand 6PH L 4113

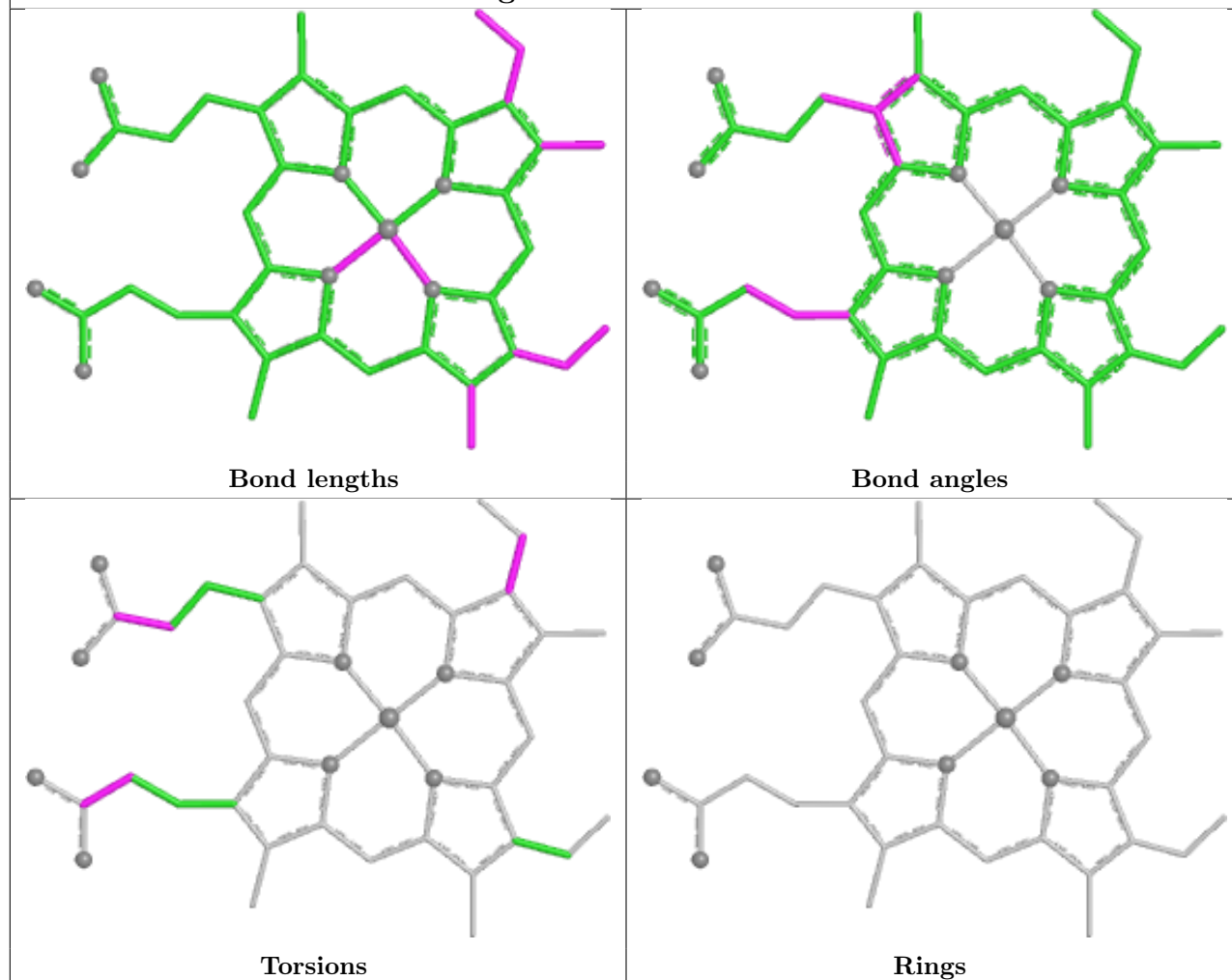


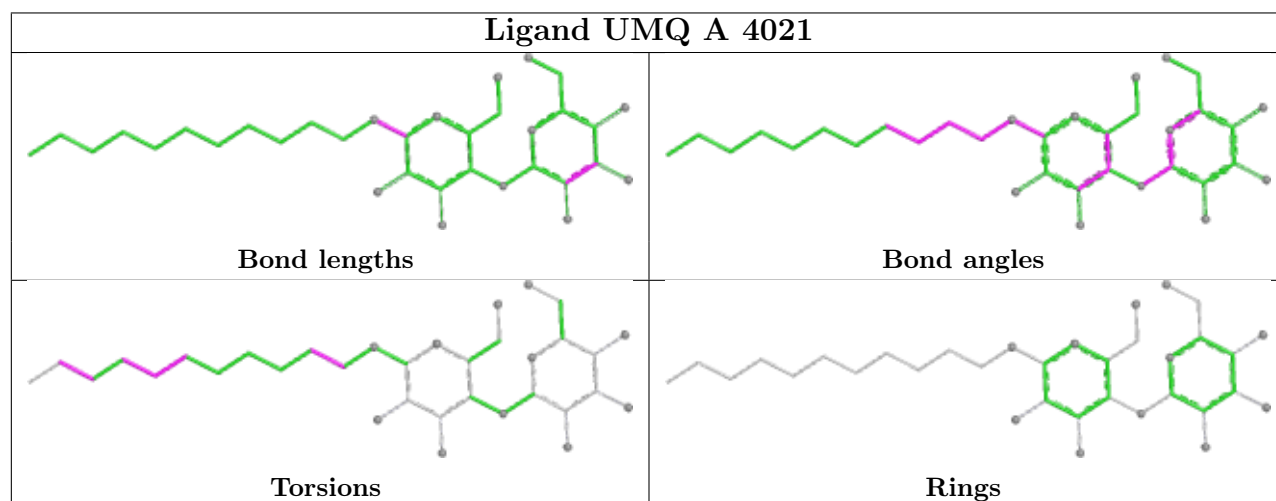
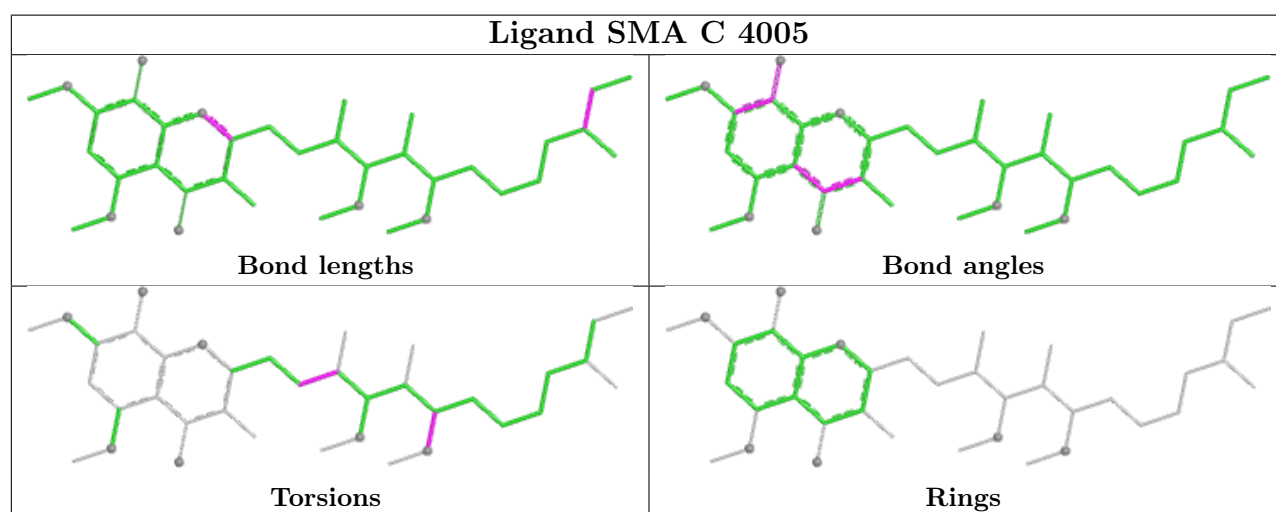
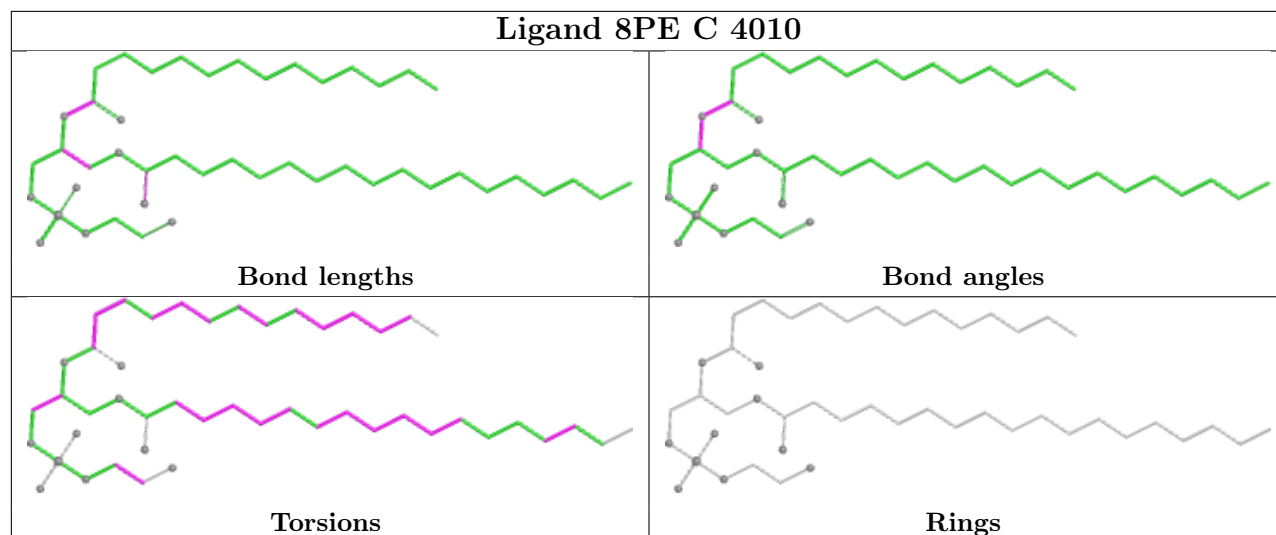


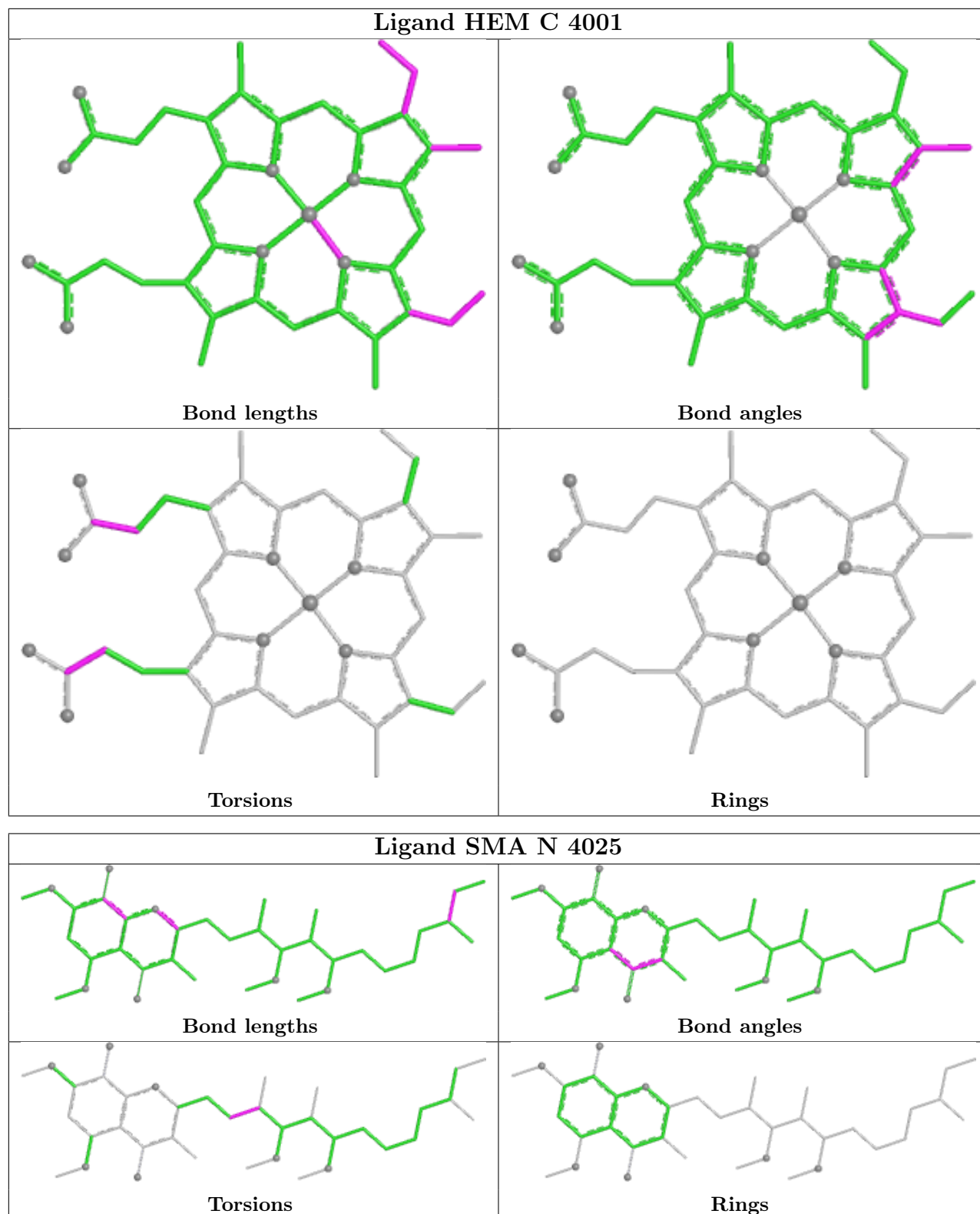
Ligand CN6 C 4031



Ligand HEM N 4021







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	431/431 (100%)	0.56	50 (11%) 9 8	32, 57, 121, 146	0
1	L	431/431 (100%)	0.45	50 (11%) 9 8	29, 53, 114, 140	0
2	B	352/352 (100%)	0.80	39 (11%) 10 8	40, 61, 101, 148	0
2	M	352/352 (100%)	0.75	36 (10%) 12 10	40, 59, 93, 137	0
3	C	385/385 (100%)	-0.38	6 (1%) 70 67	26, 35, 49, 113	0
3	N	385/385 (100%)	-0.43	6 (1%) 70 67	25, 33, 46, 104	0
4	D	246/248 (99%)	-0.04	6 (2%) 59 55	32, 48, 70, 79	0
4	O	246/248 (99%)	-0.24	4 (1%) 70 67	25, 42, 64, 80	0
5	E	185/185 (100%)	0.31	11 (5%) 28 24	32, 54, 90, 117	0
5	P	185/185 (100%)	0.18	10 (5%) 31 27	34, 52, 92, 114	0
6	F	74/146 (50%)	0.83	8 (10%) 11 9	44, 62, 112, 114	0
6	Q	74/146 (50%)	0.50	5 (6%) 23 20	39, 57, 108, 110	0
7	G	125/126 (99%)	-0.03	3 (2%) 59 55	32, 45, 72, 92	0
7	R	125/126 (99%)	-0.07	2 (1%) 70 67	28, 42, 69, 88	0
8	H	93/93 (100%)	1.07	23 (24%) 2 1	29, 57, 147, 154	0
8	S	93/93 (100%)	1.25	24 (25%) 1 1	26, 55, 154, 160	0
9	I	55/65 (84%)	0.70	6 (10%) 10 9	41, 56, 111, 124	0
9	T	55/65 (84%)	0.63	7 (12%) 8 6	37, 49, 112, 124	0
10	J	127/127 (100%)	1.17	19 (14%) 5 4	50, 74, 93, 99	0
10	U	127/127 (100%)	1.13	16 (12%) 8 6	52, 74, 89, 97	0
11	K	107/107 (100%)	2.30	58 (54%) 0 0	70, 105, 135, 141	0
11	V	107/107 (100%)	2.10	51 (47%) 0 0	72, 104, 133, 136	0
12	W	111/112 (99%)	1.01	12 (10%) 11 9	25, 70, 108, 136	1 (0%)
All	All	4471/4642 (96%)	0.43	452 (10%) 12 10	25, 53, 111, 160	1 (0%)

All (452) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	S	40	ILE	9.6
1	A	230	LEU	9.0
1	L	230	LEU	8.1
2	M	338	LEU	8.0
8	S	46	PHE	8.0
9	T	58	ALA	7.9
1	L	27	ALA	7.8
1	A	27	ALA	7.4
9	T	57	ALA	7.3
2	B	343	VAL	7.3
8	S	43	ASN	6.9
8	H	46	PHE	6.9
2	M	336	ILE	6.8
2	B	338	LEU	6.7
2	M	343	VAL	6.5
12	W	1	ALA	6.4
8	S	39	GLY	6.3
3	N	383	VAL	6.2
8	S	45	VAL	6.1
11	K	15	LEU	6.0
1	L	128	LYS	6.0
3	N	384	ASN	5.9
1	A	228	LEU	5.8
1	A	237	VAL	5.8
2	B	332	VAL	5.8
3	N	385	LYS	5.8
2	M	314	LEU	5.7
3	C	346	VAL	5.6
9	I	57	ALA	5.6
1	A	124	PHE	5.6
2	B	336	ILE	5.6
3	N	346	VAL	5.6
8	S	94	VAL	5.6
8	S	51	ARG	5.5
9	I	58	ALA	5.4
11	K	4	LEU	5.3
2	B	334	SER	5.3
1	L	234	THR	5.3
2	M	311	GLY	5.3
9	T	56	ILE	5.3
2	B	333	SER	5.2
2	B	215	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
8	S	44	ALA	5.2
12	W	5	THR	5.1
8	S	41	PHE	5.1
1	L	31	GLN	5.1
1	L	237	VAL	5.1
1	A	31	GLN	5.0
1	A	125	ILE	5.0
2	B	331	SER	5.0
8	H	5	SER	5.0
3	C	383	VAL	5.0
11	K	9	VAL	5.0
12	W	4	SER	4.9
3	C	385	LYS	4.9
1	L	228	LEU	4.9
11	V	9	VAL	4.9
1	L	213	ASN	4.9
1	A	35	GLY	4.9
2	M	312	LYS	4.9
11	K	75	ILE	4.8
8	H	94	VAL	4.8
8	S	68	TYR	4.8
8	S	50	ARG	4.7
11	K	21	ILE	4.7
1	A	128	LYS	4.7
11	K	11	LEU	4.7
11	V	11	LEU	4.7
10	U	42	PRO	4.6
11	V	80	PRO	4.6
8	H	40	ILE	4.6
1	L	231	GLN	4.5
2	B	313	ASP	4.5
11	K	35	TRP	4.5
11	K	23	CYS	4.4
8	H	45	VAL	4.4
1	L	124	PHE	4.4
2	M	340	PHE	4.3
8	H	41	PHE	4.3
11	K	80	PRO	4.3
1	A	236	PRO	4.3
2	M	327	VAL	4.3
1	L	34	ASN	4.3
8	H	37	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
8	S	49	PHE	4.2
1	A	229	SER	4.2
9	I	56	ILE	4.2
11	K	2	ILE	4.2
11	K	69	THR	4.2
1	A	28	GLU	4.2
8	H	51	ARG	4.2
8	S	42	HIS	4.2
1	L	271	ASN	4.2
11	K	7	THR	4.1
3	C	384	ASN	4.1
2	B	312	LYS	4.1
8	S	37	LEU	4.1
11	V	106	ILE	4.0
11	K	33	LEU	4.0
2	B	335	PRO	4.0
8	H	49	PHE	4.0
1	L	214	ILE	4.0
1	A	213	ASN	4.0
11	K	16	GLY	4.0
6	Q	117	LEU	4.0
11	K	13	ALA	3.9
11	V	4	LEU	3.9
8	H	42	HIS	3.9
1	A	401	LEU	3.9
1	L	35	GLY	3.9
8	S	2	GLY	3.9
4	D	67	HIS	3.9
1	A	231	GLN	3.9
10	J	68	LEU	3.9
8	H	48	SER	3.9
1	L	30	THR	3.8
8	H	43	ASN	3.8
11	V	83	ILE	3.8
2	M	344	LYS	3.8
8	H	52	PHE	3.8
12	W	7	PHE	3.8
2	B	154	GLY	3.8
11	K	83	ILE	3.8
2	B	328	GLN	3.8
10	U	87	THR	3.7
11	V	19	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	340	PHE	3.7
1	L	33	SER	3.7
2	B	249	SER	3.7
10	J	31	SER	3.7
11	K	19	VAL	3.7
1	L	42	HIS	3.7
1	A	214	ILE	3.7
11	V	100	ALA	3.7
1	A	36	ILE	3.7
11	V	2	ILE	3.7
11	V	73	LEU	3.7
11	V	107	LYS	3.6
2	B	329	ASN	3.6
1	A	234	THR	3.6
8	S	52	PHE	3.6
11	K	8	PRO	3.6
1	A	34	ASN	3.6
1	A	29	VAL	3.6
1	L	29	VAL	3.6
1	A	127	GLN	3.6
2	M	313	ASP	3.6
10	J	30	THR	3.5
2	M	212	GLY	3.5
11	V	29	ILE	3.5
11	K	92	ILE	3.5
1	L	127	GLN	3.5
11	V	7	THR	3.5
12	W	2	LYS	3.5
11	V	21	ILE	3.4
8	S	47	ASN	3.4
12	W	6	GLY	3.4
2	M	342	ALA	3.4
5	E	103	LEU	3.4
8	H	44	ALA	3.4
11	K	58	VAL	3.4
11	V	78	LEU	3.4
8	S	4	PRO	3.4
11	V	75	ILE	3.3
8	S	54	SER	3.3
1	A	30	THR	3.3
9	I	54	ALA	3.3
12	W	12	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
8	H	38	GLN	3.3
2	M	329	ASN	3.3
11	V	15	LEU	3.3
4	D	140	GLU	3.3
10	U	29	ILE	3.3
8	S	48	SER	3.3
5	E	47	ASN	3.3
11	V	92	ILE	3.3
1	L	129	ALA	3.3
6	F	111	GLN	3.2
11	V	8	PRO	3.2
11	V	23	CYS	3.2
2	M	330	GLU	3.2
1	L	32	LEU	3.2
2	M	332	VAL	3.2
11	K	29	ILE	3.2
1	A	33	SER	3.2
2	M	83	ASP	3.2
1	A	134	SER	3.2
1	A	46	ALA	3.1
1	L	236	PRO	3.1
11	V	30	ASN	3.1
11	K	20	THR	3.1
6	Q	119	HIS	3.1
1	A	381	GLY	3.1
6	F	74	VAL	3.1
10	U	32	GLY	3.1
2	B	321	THR	3.1
2	M	310	LYS	3.1
9	T	4	SER	3.1
8	H	47	ASN	3.1
2	B	250	LEU	3.1
2	M	328	GLN	3.0
8	H	68	TYR	3.0
1	A	380	SER	3.0
2	M	331	SER	3.0
8	H	6	GLY	3.0
11	K	96	TRP	3.0
1	L	232	THR	3.0
11	V	5	THR	3.0
1	L	229	SER	3.0
1	L	125	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	314	LEU	3.0
6	F	117	LEU	3.0
5	P	49	ALA	3.0
2	B	155	LEU	3.0
11	K	12	ALA	2.9
12	W	22[A]	ARG	2.9
8	H	2	GLY	2.9
1	A	232	THR	2.9
1	A	238	LEU	2.9
2	B	311	GLY	2.9
1	L	238	LEU	2.9
11	V	96	TRP	2.9
11	K	22	SER	2.9
7	R	127	LYS	2.9
10	J	124	TRP	2.9
11	V	17	ASP	2.9
1	L	233	GLY	2.9
11	V	26	SER	2.8
2	B	248	ALA	2.8
11	K	27	GLN	2.8
11	K	70	ASP	2.8
1	A	225	SER	2.8
11	K	26	SER	2.8
5	E	94	VAL	2.8
9	T	54	ALA	2.8
2	M	292	GLN	2.8
10	U	124	TRP	2.8
2	B	318	ILE	2.8
2	B	327	VAL	2.8
10	U	114	GLN	2.8
8	S	67	TRP	2.8
10	U	10	GLY	2.8
1	L	36	ILE	2.8
11	K	71	TYR	2.8
11	K	65	SER	2.8
10	U	64	LEU	2.8
1	A	271	ASN	2.7
5	P	47	ASN	2.7
11	K	30	ASN	2.7
2	B	214	SER	2.7
2	M	315	SER	2.7
9	T	12	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	126	GLN	2.7
11	K	44	ILE	2.7
10	J	18	LEU	2.7
11	V	24	ARG	2.7
2	B	330	GLU	2.7
6	Q	118	GLU	2.7
10	U	38	ILE	2.7
8	S	53	LYS	2.7
11	V	104	LEU	2.7
5	E	49	ALA	2.7
2	B	293	ASP	2.6
2	B	212	GLY	2.6
1	A	400	LYS	2.6
2	B	344	LYS	2.6
10	J	62	PRO	2.6
2	B	339	ASN	2.6
10	J	122	SER	2.6
11	V	3	GLU	2.6
2	B	317	ALA	2.6
11	K	5	THR	2.6
11	V	51	THR	2.6
12	W	50	GLY	2.6
11	K	106	ILE	2.6
2	M	250	LEU	2.6
1	L	217	GLU	2.6
11	V	71	TYR	2.6
4	O	286	TRP	2.6
2	M	267	LEU	2.6
11	K	93	LYS	2.6
1	L	28	GLU	2.6
11	K	73	LEU	2.6
2	M	136	GLN	2.6
6	F	75	THR	2.6
2	B	345	ASP	2.5
2	M	337	GLU	2.5
10	J	11	LEU	2.5
5	E	46	ASN	2.5
1	L	226	LYS	2.5
11	V	40	PRO	2.5
1	L	131	LEU	2.5
11	V	32	PHE	2.5
1	L	134	SER	2.5

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Mol	Chain	Res	Type	RSRZ
11	K	102	THR	2.5
2	M	335	PRO	2.5
2	M	341	ASP	2.5
4	O	170	GLN	2.5
4	D	185	HIS	2.5
11	K	31	ASN	2.5
2	M	334	SER	2.5
10	U	30	THR	2.5
8	H	39	GLY	2.5
11	V	42	GLY	2.5
11	V	70	ASP	2.5
1	L	240	LYS	2.5
11	K	103	LYS	2.5
5	P	124	HIS	2.5
5	E	97	ASN	2.5
11	K	10	SER	2.5
11	V	14	SER	2.5
11	K	62	PHE	2.4
1	L	220	VAL	2.4
2	M	246	ASN	2.4
11	V	10	SER	2.4
6	Q	112	PRO	2.4
11	V	16	GLY	2.4
1	A	126	GLN	2.4
6	F	119	HIS	2.4
5	P	42	VAL	2.4
1	A	239	LYS	2.4
2	B	310	LYS	2.4
1	A	219	LEU	2.4
1	L	219	LEU	2.4
11	K	104	LEU	2.4
5	E	100	ALA	2.4
11	K	56	ALA	2.4
4	O	235	GLU	2.4
11	K	51	THR	2.4
1	L	76	ILE	2.4
6	F	107	ILE	2.4
1	A	209	VAL	2.4
1	A	227	ASN	2.4
1	L	123	SER	2.3
2	B	360	SER	2.3
11	V	65	SER	2.3

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Mol	Chain	Res	Type	RSRZ
7	G	123	ILE	2.3
11	K	24	ARG	2.3
11	K	86	TYR	2.3
1	A	235	LYS	2.3
6	F	112	PRO	2.3
11	V	20	THR	2.3
9	T	55	ARG	2.3
11	K	63	SER	2.3
2	M	318	ILE	2.3
7	G	66	ASP	2.3
11	V	88	CYS	2.3
1	A	220	VAL	2.3
2	B	337	GLU	2.3
11	V	81	GLU	2.3
1	L	46	ALA	2.3
8	S	84	ALA	2.3
10	U	93	THR	2.3
1	A	79	SER	2.3
2	M	214	SER	2.3
11	K	14	SER	2.3
11	V	72	SER	2.3
1	L	424	LYS	2.3
12	W	8	LYS	2.3
6	Q	114	TYR	2.3
9	I	13	ARG	2.3
1	A	123	SER	2.3
9	I	4	SER	2.3
10	U	63	SER	2.3
10	J	64	LEU	2.3
10	J	87	THR	2.2
10	J	32	GLY	2.2
1	L	45	SER	2.2
10	J	63	SER	2.2
2	B	151	PHE	2.2
8	H	86	ARG	2.2
1	L	63	ASN	2.2
2	B	315	SER	2.2
10	J	70	ILE	2.2
11	K	81	GLU	2.2
3	C	347	PRO	2.2
7	R	125	VAL	2.2
1	L	239	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	400	LYS	2.2
11	K	78	LEU	2.2
11	V	68	GLY	2.2
3	C	223	SER	2.2
10	U	75	SER	2.2
10	U	99	SER	2.2
1	A	224	GLU	2.2
8	H	67	TRP	2.2
10	J	42	PRO	2.2
1	L	88	LYS	2.2
5	E	124	HIS	2.2
10	J	123	ALA	2.2
11	K	6	GLN	2.2
6	F	114	TYR	2.2
10	J	93	THR	2.2
2	M	333	SER	2.2
8	H	50	ARG	2.2
11	K	107	LYS	2.2
2	M	339	ASN	2.1
1	A	180	GLY	2.1
1	A	233	GLY	2.1
12	W	10	GLY	2.1
10	J	19	SER	2.1
11	V	18	ARG	2.1
11	V	76	SER	2.1
1	A	240	LYS	2.1
8	S	3	PRO	2.1
11	V	27	GLN	2.1
2	B	211	ALA	2.1
11	K	74	THR	2.1
11	V	69	THR	2.1
1	L	150	ASP	2.1
1	L	380	SER	2.1
2	B	292	GLN	2.1
7	G	20	VAL	2.1
4	D	286	TRP	2.1
1	A	132	LEU	2.1
4	D	239	GLY	2.1
11	V	33	LEU	2.1
5	P	213	ILE	2.1
1	L	115	LYS	2.1
1	L	215	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	122	GLN	2.1
5	E	214	VAL	2.1
5	P	90	ALA	2.1
11	K	25	ALA	2.1
5	P	46	ASN	2.1
5	E	213	ILE	2.1
11	V	103	LYS	2.1
11	V	28	ASP	2.1
10	U	55	VAL	2.0
1	A	84	ALA	2.0
11	K	64	GLY	2.0
11	K	101	GLY	2.0
2	M	366	ASP	2.0
5	P	210	ASP	2.0
10	U	66	ASP	2.0
1	A	45	SER	2.0
2	M	360	SER	2.0
3	N	347	PRO	2.0
4	O	307	PRO	2.0
11	K	72	SER	2.0
12	W	25	GLN	2.0
5	P	96	VAL	2.0
2	M	211	ALA	2.0
5	E	98	LEU	2.0
5	P	44	LYS	2.0
10	J	100	GLU	2.0
10	J	106	GLY	2.0
11	V	45	LYS	2.0
1	A	457	TRP	2.0
11	K	59	PRO	2.0
3	N	223	SER	2.0
4	D	70	HIS	2.0

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

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

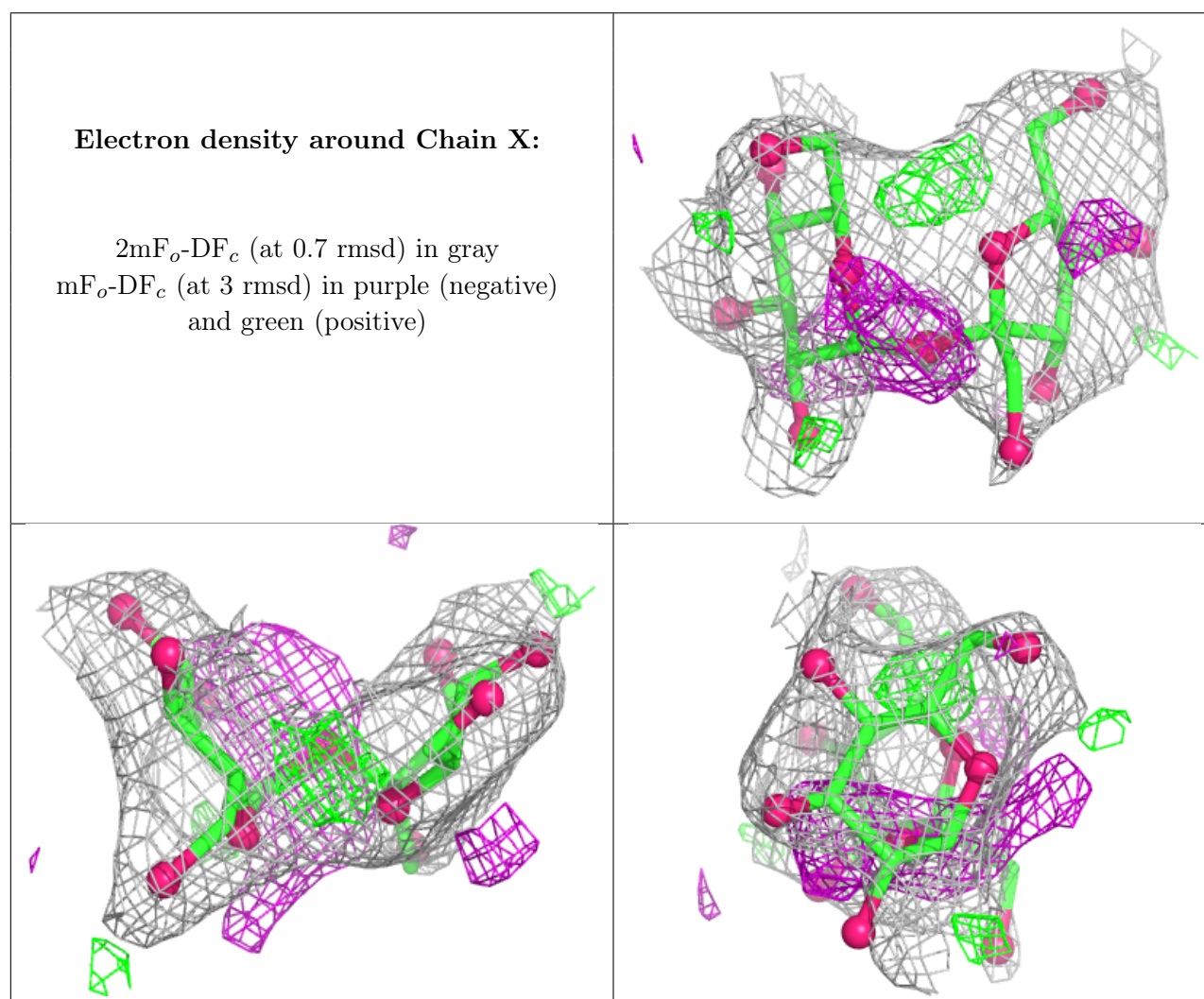
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	M3L	W	81	12/13	0.86	0.13	60,63,64,66	0

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	FRU	X	2	12/12	0.75	0.19	77,79,81,81	0
13	GLC	X	1	11/12	0.80	0.20	72,75,77,78	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

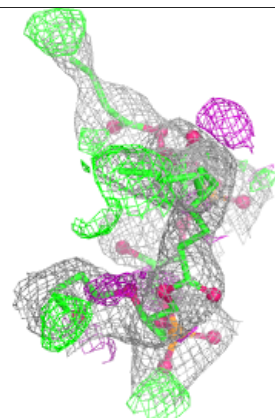
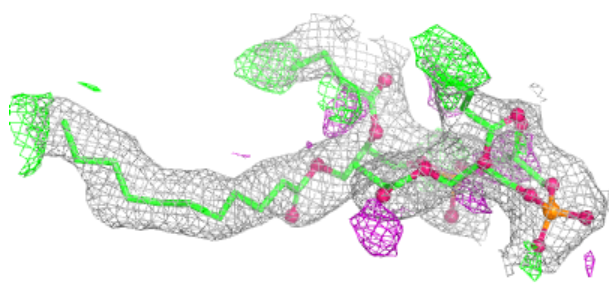
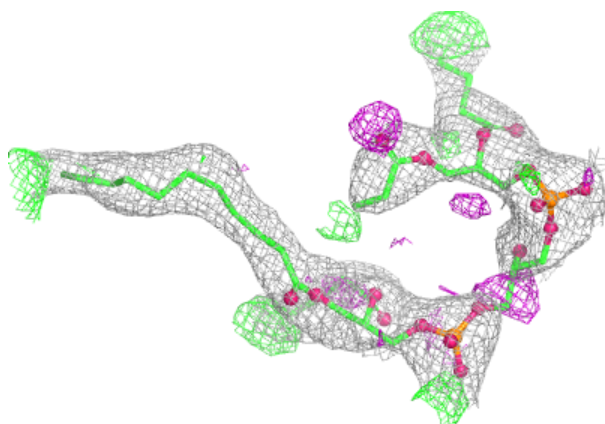
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	CN6	N	4131	50/50	0.85	0.18	53,67,77,79	0
22	6PH	E	4013	40/40	0.85	0.15	56,65,72,72	0
22	6PH	L	4113	40/40	0.85	0.15	49,60,69,69	0
18	CN6	C	4031	50/50	0.86	0.18	50,70,78,80	0
19	9PE	C	4111	40/40	0.87	0.14	45,57,75,76	0
17	8PE	N	4110	47/47	0.89	0.15	28,65,74,75	0
17	8PE	C	4010	47/47	0.89	0.13	39,59,62,65	0
19	9PE	N	4011	40/40	0.90	0.13	50,54,63,64	0
14	UMQ	A	4021	34/34	0.91	0.10	42,48,65,67	0
14	UMQ	L	4121	34/34	0.91	0.10	39,44,59,60	0
20	7PH	D	4014	38/38	0.92	0.10	48,53,61,62	0
20	7PH	O	4114	38/38	0.93	0.09	38,44,51,54	0
15	HEM	W	4026	43/43	0.96	0.10	47,55,57,58	0
16	SMA	N	4025	37/37	0.96	0.06	23,28,31,32	0
16	SMA	C	4005	37/37	0.97	0.06	29,33,37,37	0
15	HEM	D	4003	43/43	0.98	0.06	35,39,43,44	0
15	HEM	C	4001	43/43	0.98	0.06	21,26,32,35	0
15	HEM	N	4021	43/43	0.99	0.06	15,23,30,34	0
15	HEM	N	4022	43/43	0.99	0.05	21,23,32,35	0
21	FES	E	4004	4/4	0.99	0.02	30,32,32,37	0
21	FES	P	4024	4/4	0.99	0.02	32,36,36,37	0
15	HEM	O	4023	43/43	0.99	0.05	32,37,41,42	0
15	HEM	C	4002	43/43	0.99	0.06	20,26,37,37	0

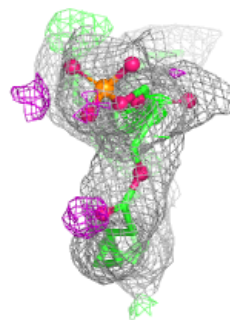
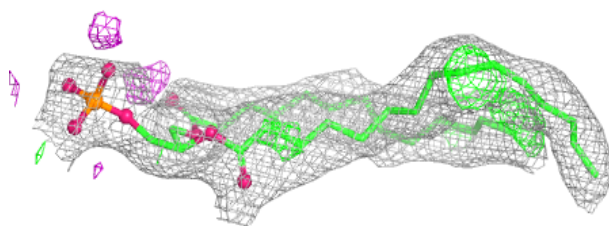
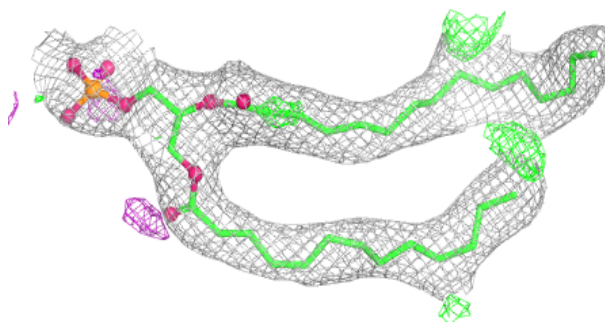
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CN6 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)

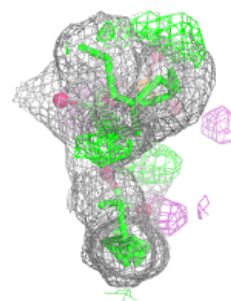
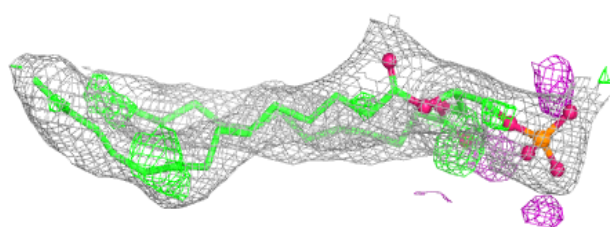
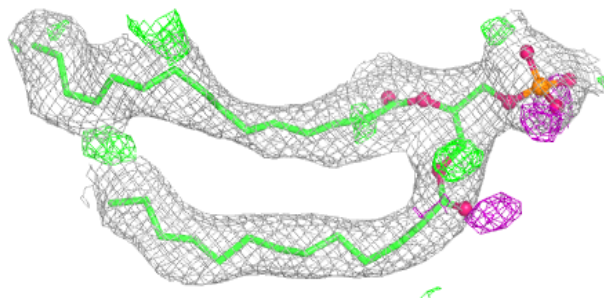
**Electron density around 6PH E 4013:**

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

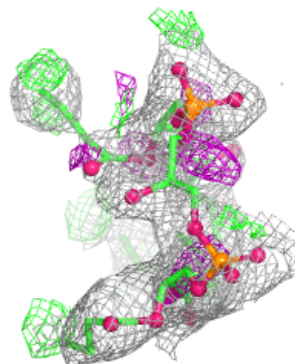
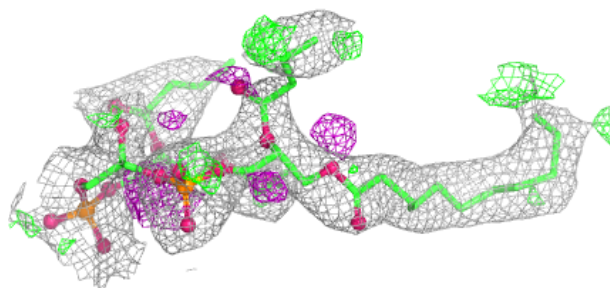
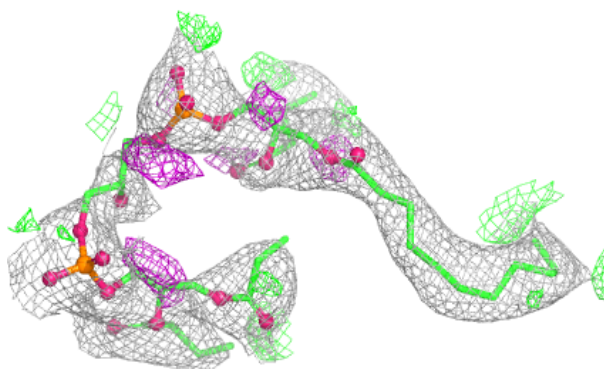


Electron density around 6PH L 4113:

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

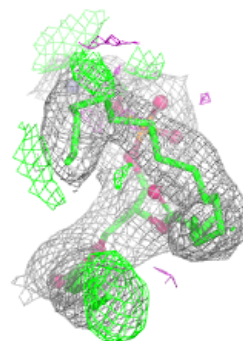
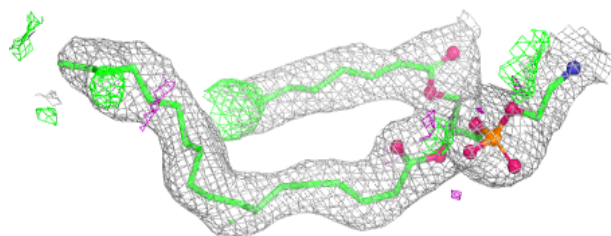
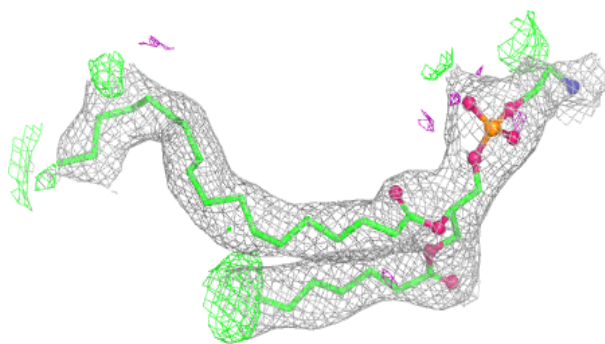
**Electron density around CN6 C 4031:**

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

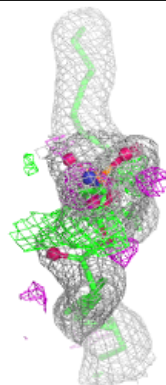
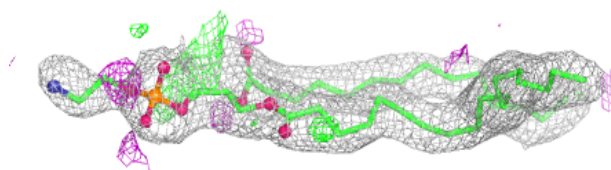
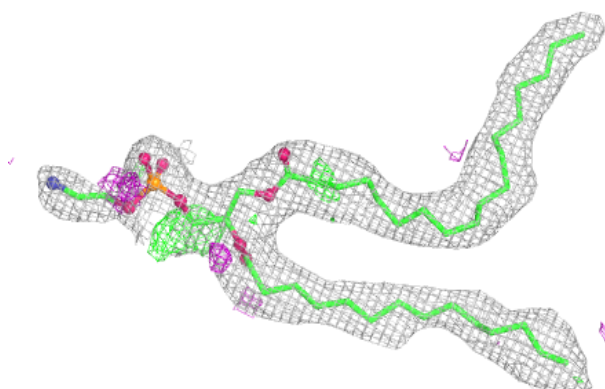


Electron density around 9PE C 4111:

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

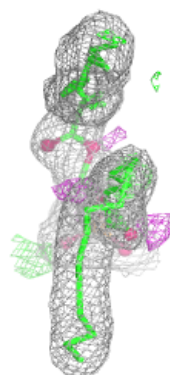
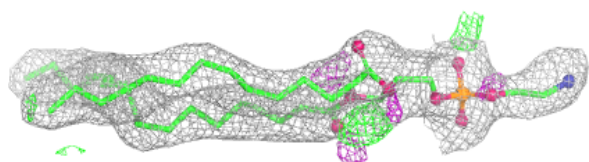
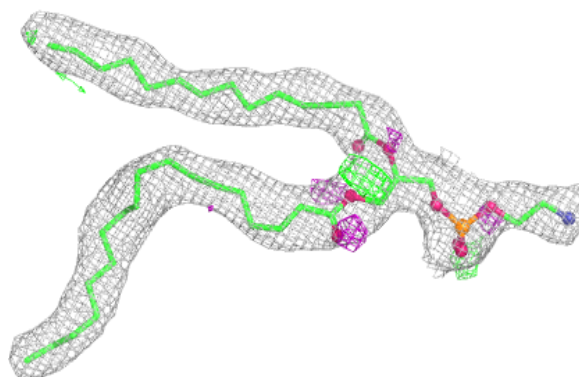
**Electron density around 8PE N 4110:**

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

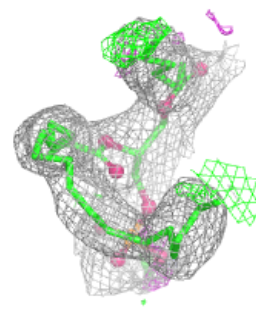
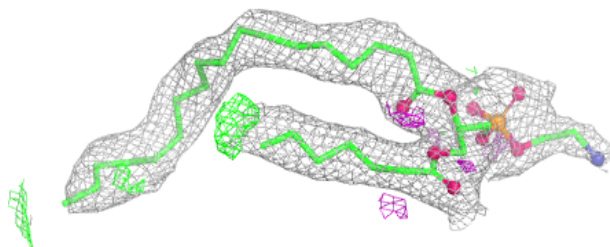
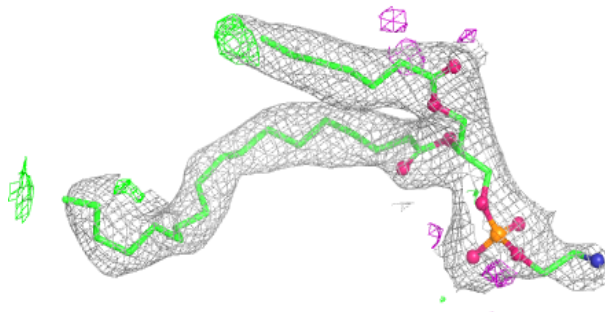


Electron density around 8PE C 4010:

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

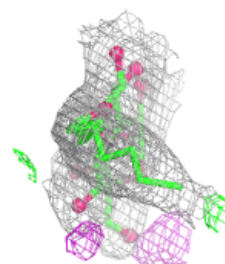
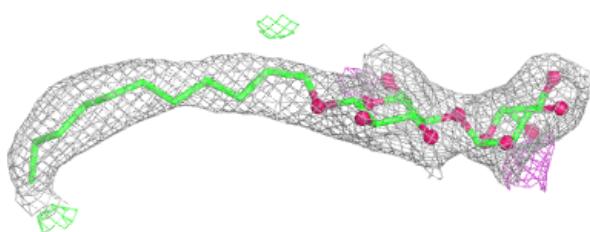
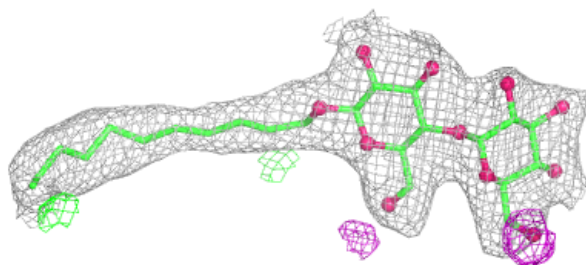
**Electron density around 9PE N 4011:**

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

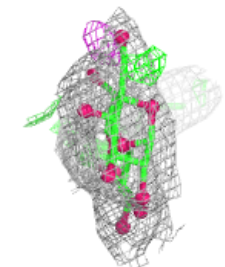
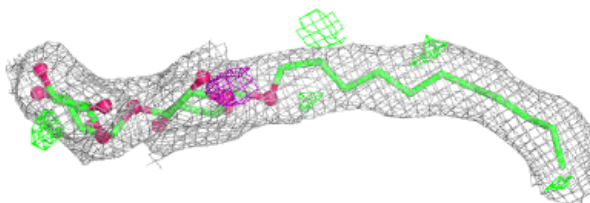
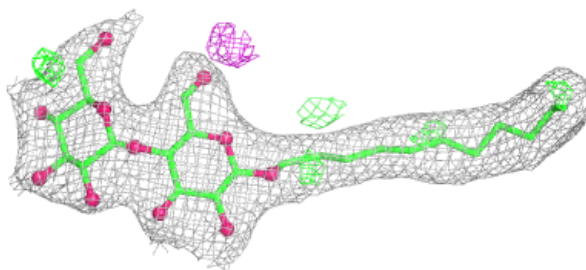


Electron density around UMQ A 4021:

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

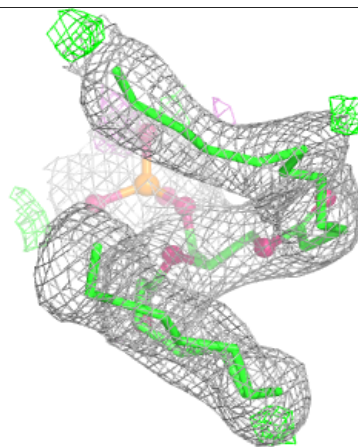
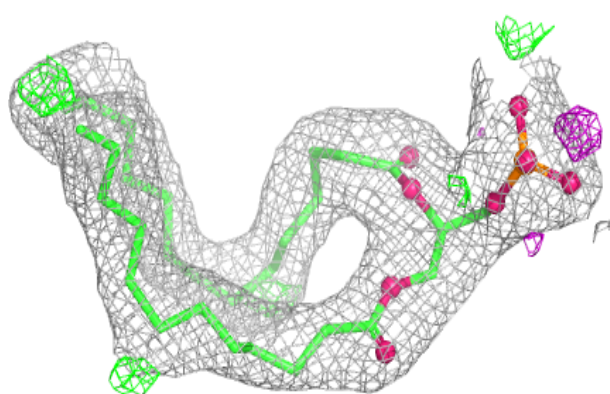
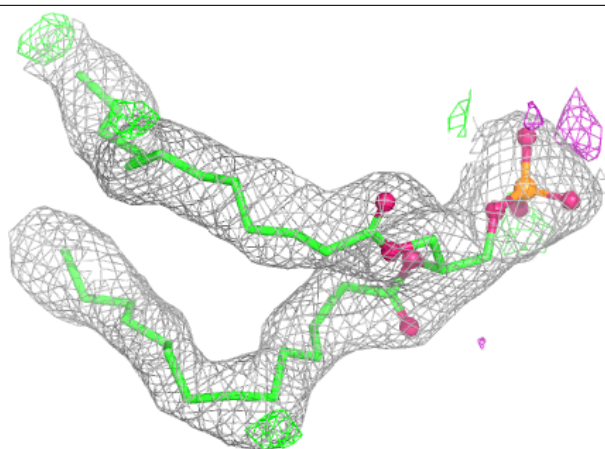
**Electron density around UMQ L 4121:**

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



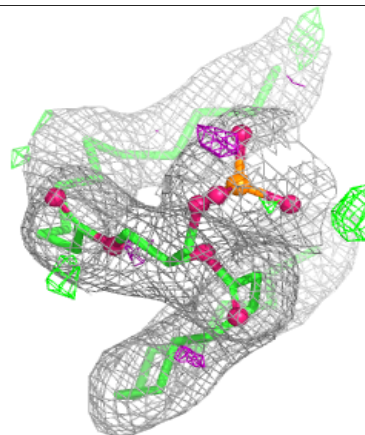
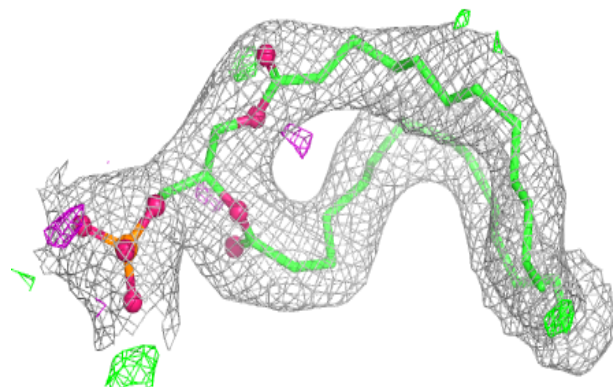
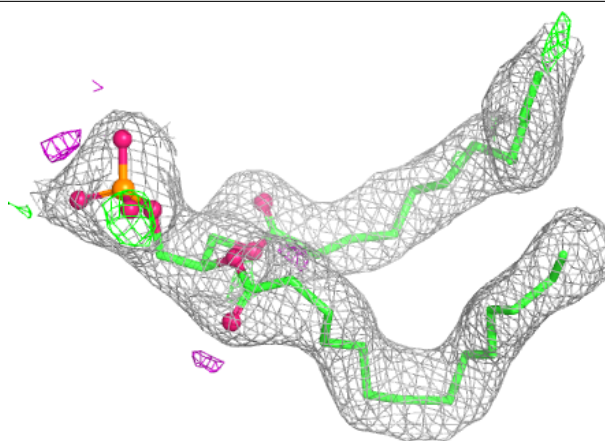
Electron density around 7PH D 4014:

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



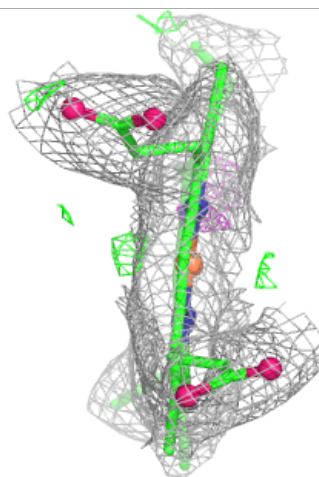
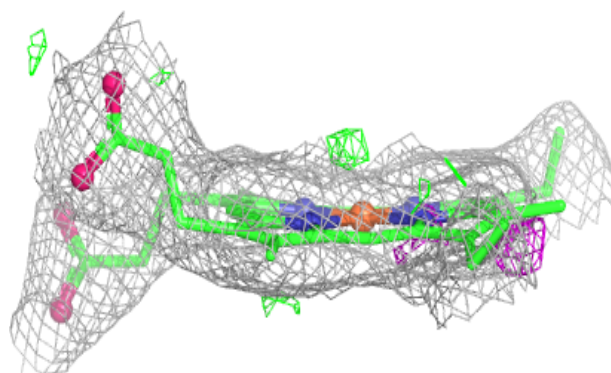
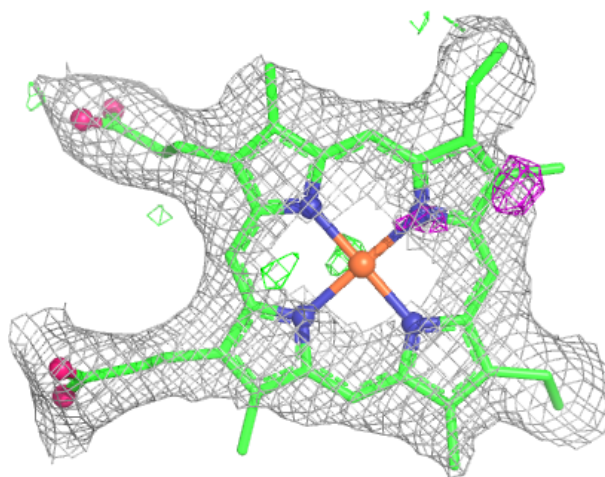
Electron density around 7PH O 4114:

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



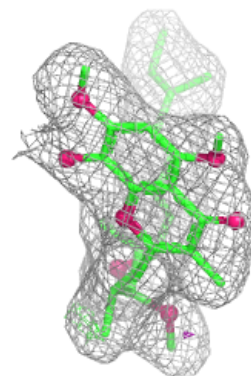
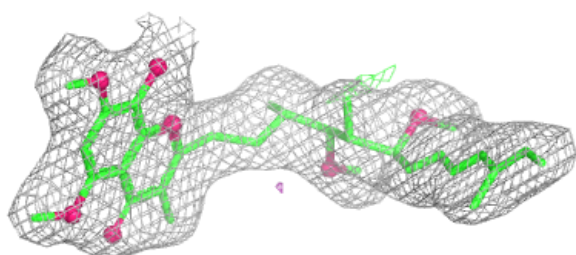
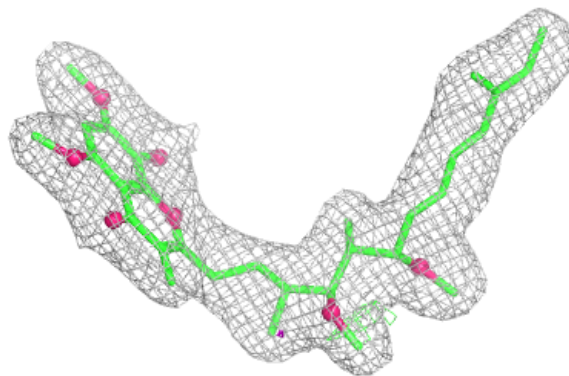
Electron density around HEM W 4026:

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



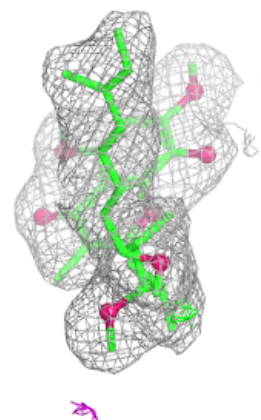
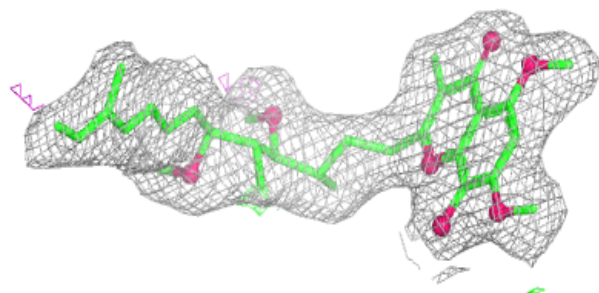
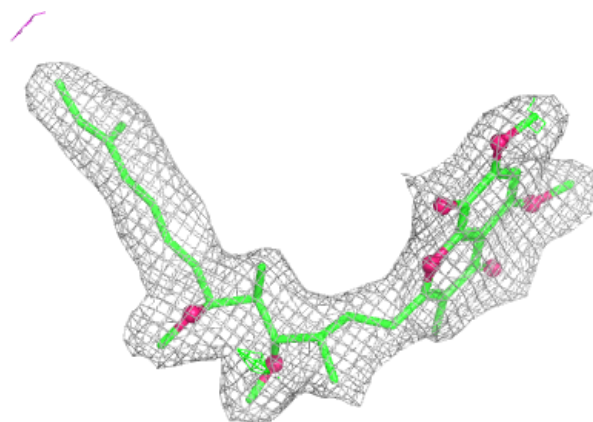
Electron density around SMA N 4025:

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



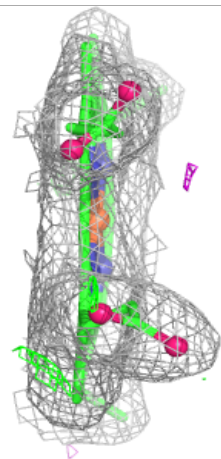
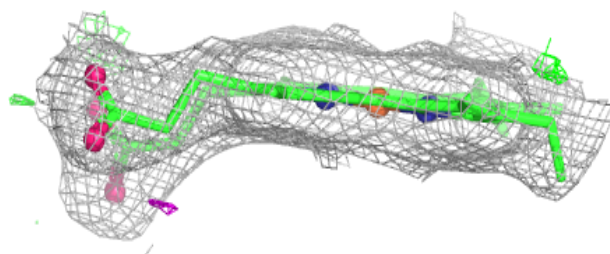
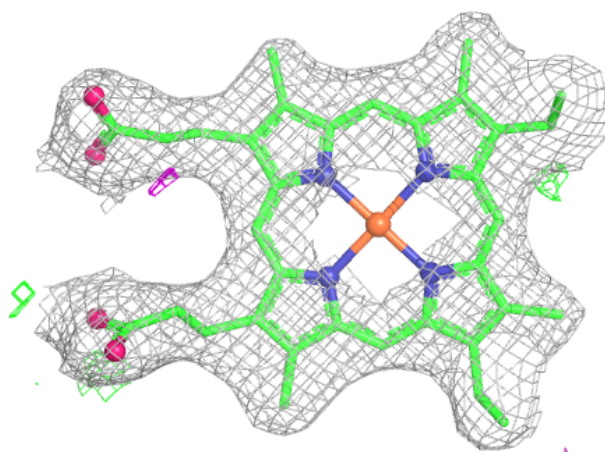
Electron density around SMA C 4005:

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



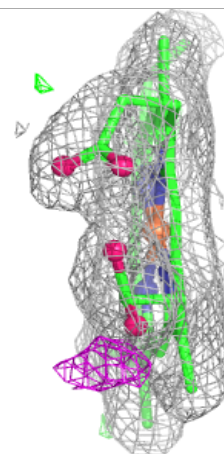
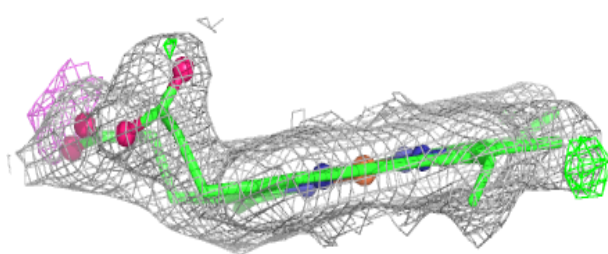
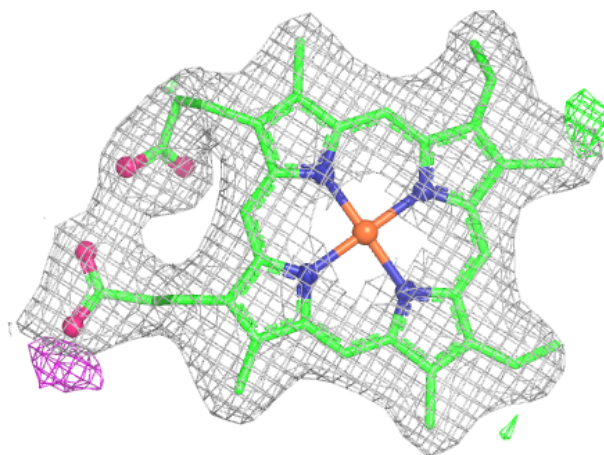
Electron density around HEM D 4003:

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



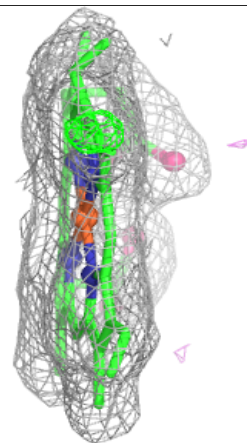
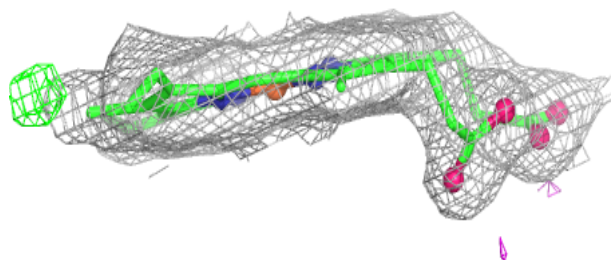
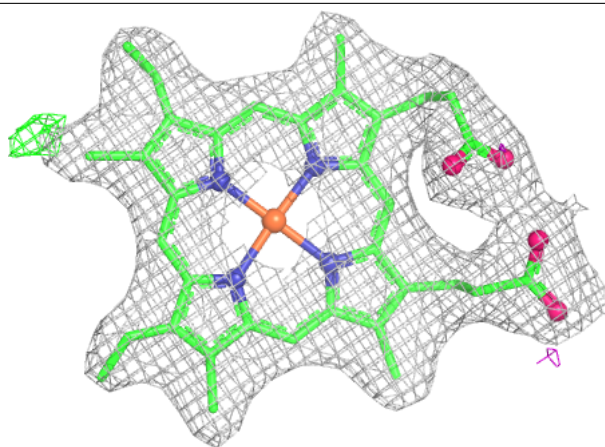
Electron density around HEM C 4001:

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



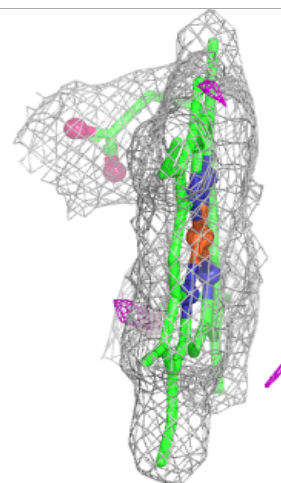
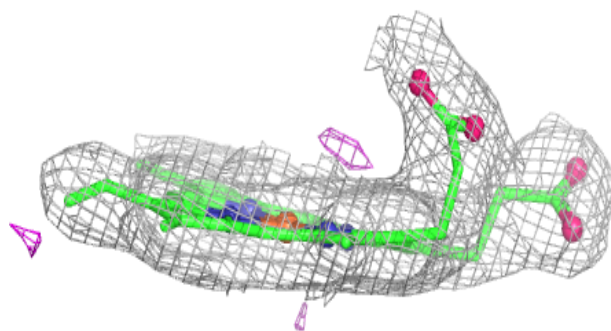
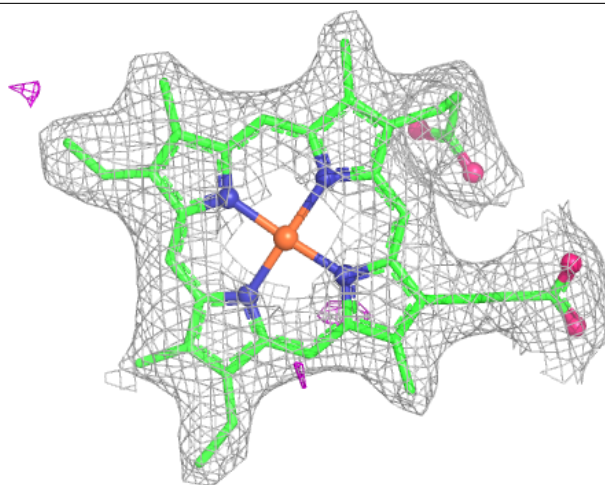
Electron density around HEM N 4021:

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



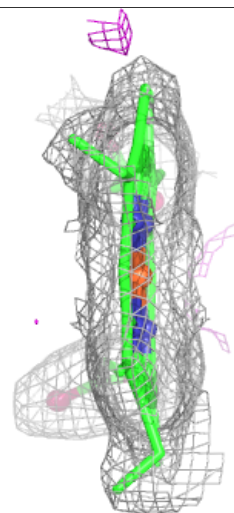
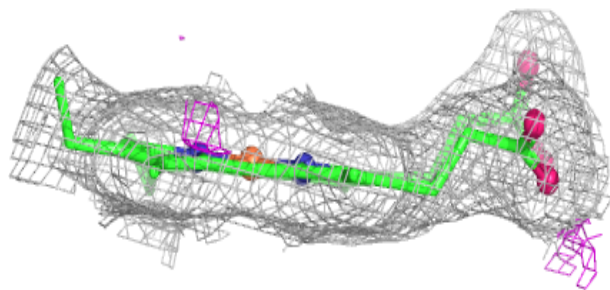
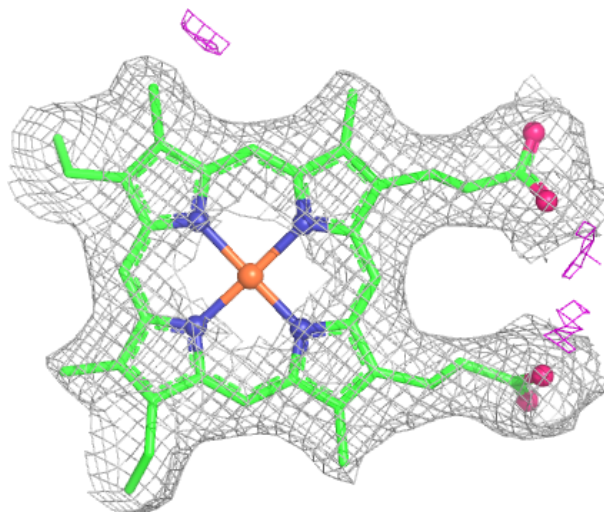
Electron density around HEM N 4022:

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



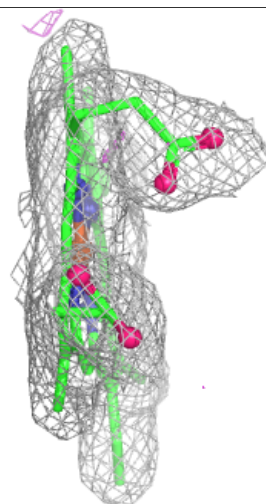
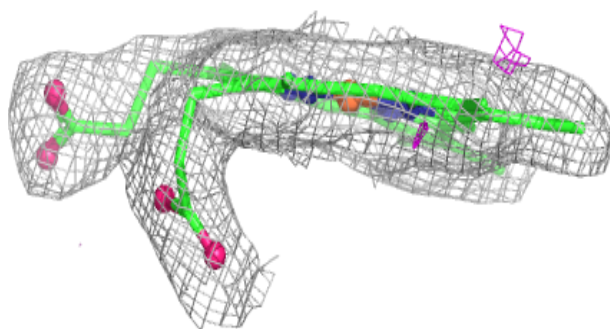
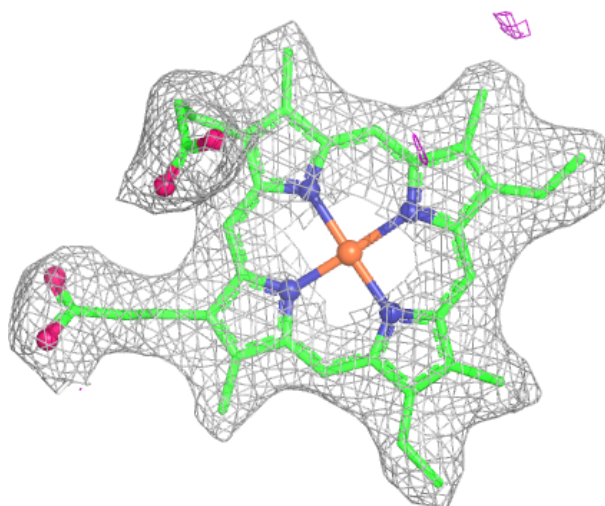
Electron density around HEM O 4023:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.