



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 03:30 PM EDT

PDB ID : 3CX5 / pdb_00003cx5
Title : Structure of complex III with bound cytochrome c in reduced state and definition of a minimal core interface for electron transfer.
Authors : Solmaz, S.R.N.; Hunte, C.
Deposited on : 2008-04-23
Resolution : 1.90 Å(reported)

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

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

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

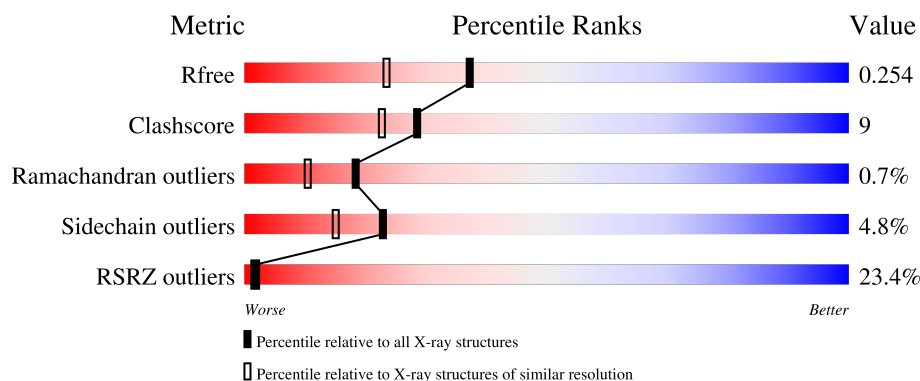
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	25% 78% 20%
1	L	431	21% 76% 21%
2	B	352	26% 76% 22%
2	M	352	26% 70% 25%
3	C	385	2% 81% 17%

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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	108	
13	X	2	

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 38020 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is a protein called CYTOCHROME B.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

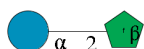
- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

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

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

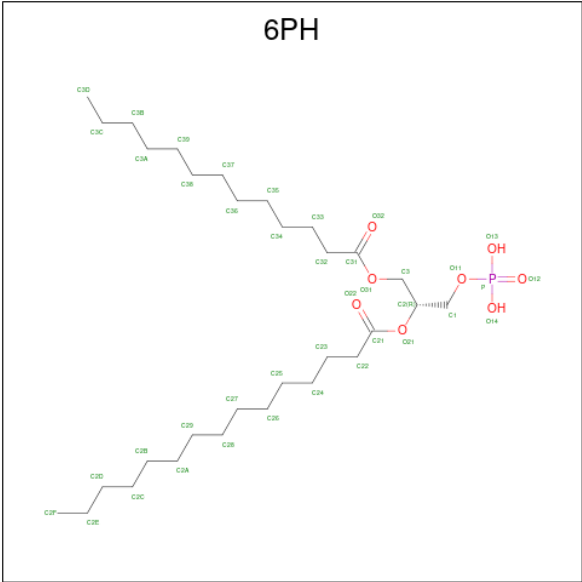
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	108	Total	C	N	O	S	0	1	0
			859	542	153	159	5			

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



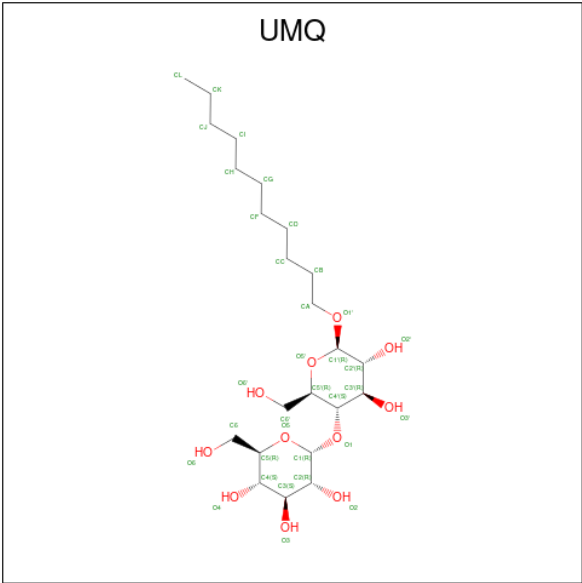
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
13	X	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 14 is (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (CCD ID: 6PH) (formula: C₃₁H₆₁O₈P).



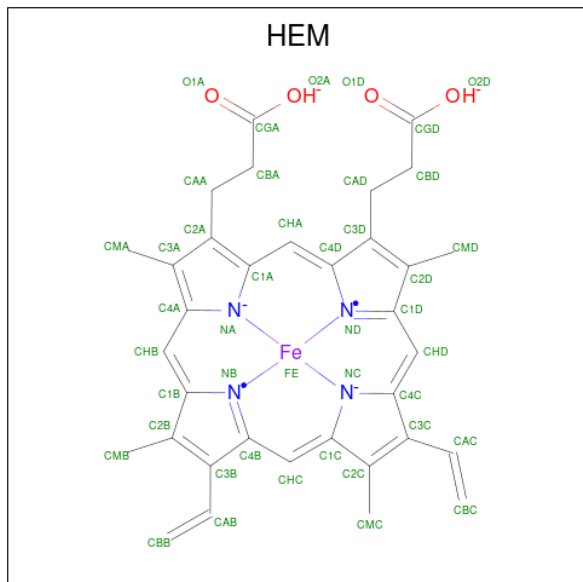
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	O	P	0	0
			40	31	8	1		
14	L	1	Total	C	O	P	0	0
			40	31	8	1		

- Molecule 15 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



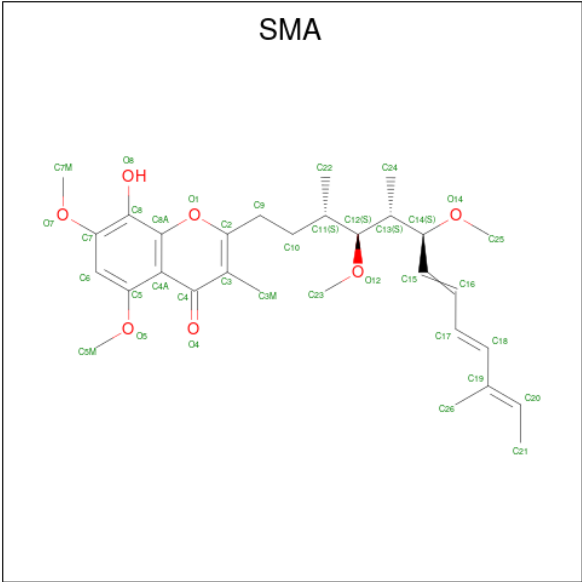
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			34	23	11		
15	L	1	Total	C	O	0	0
			34	23	11		

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



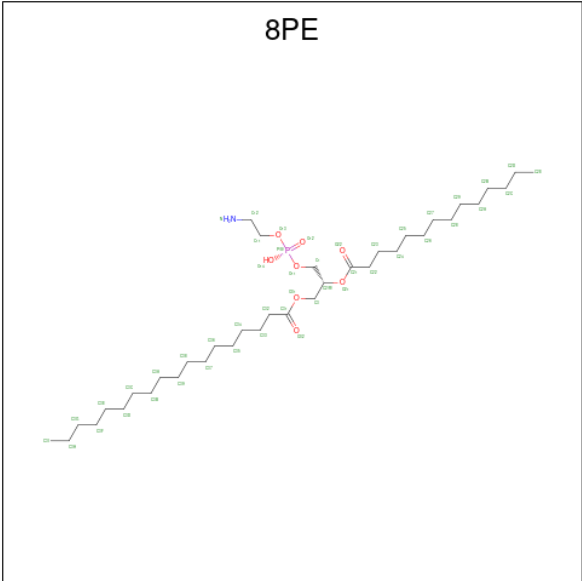
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
16	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	W	1	Total 43	C 34	Fe 1	N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

- Molecule 17 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



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

- Molecule 18 is (2R)-3-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: C₃₇H₇₄NO₈P).



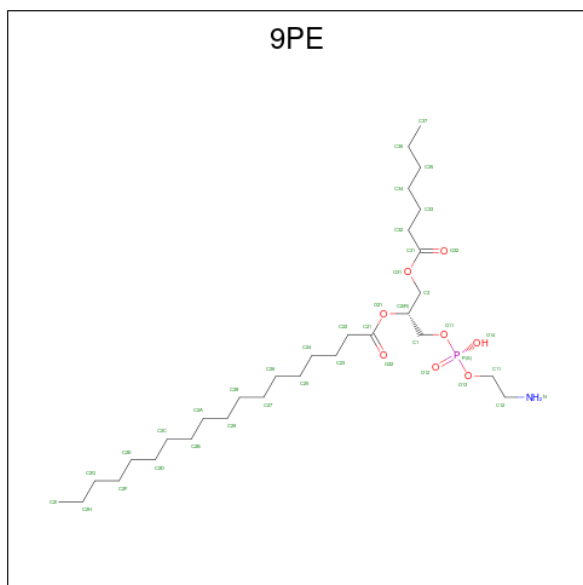
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

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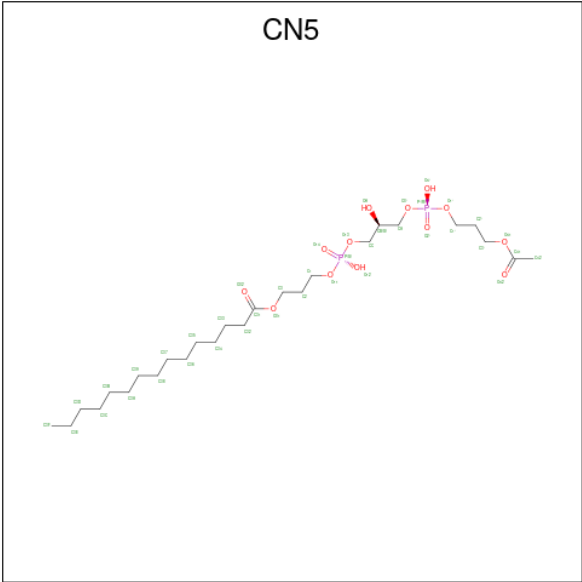
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	N	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

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



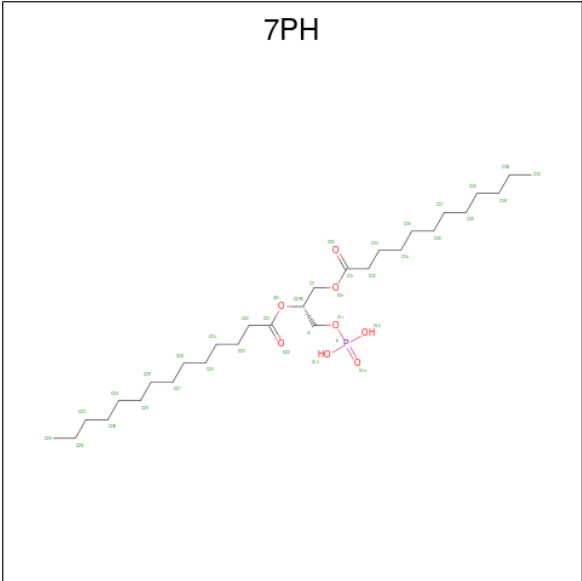
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
19	N	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 20 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-diphosphaoctadec-1-yl pentadecanoate (CCD ID: CN5) (formula: C₂₆H₅₂O₁₃P₂).



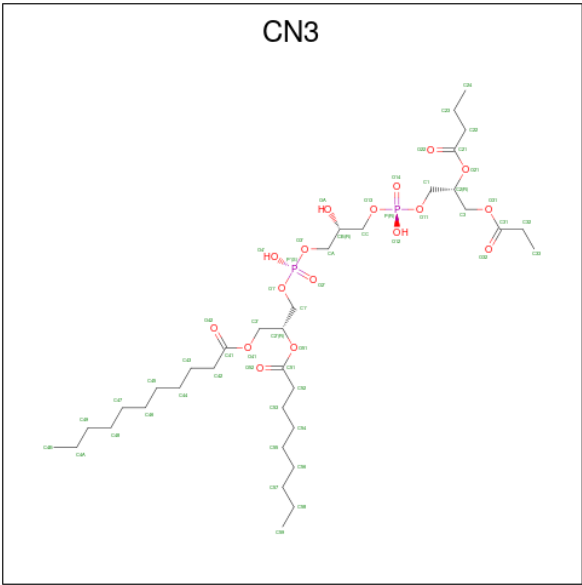
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	C	1	Total	C	O	P	0	0
			41	26	13	2		

- Molecule 21 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).



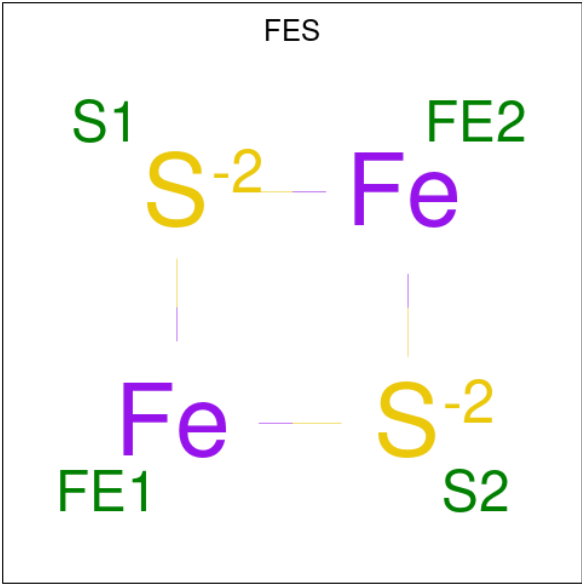
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	D	1	Total	C	O	P	0	0
			38	29	8	1		
21	O	1	Total	C	O	P	0	0
			38	29	8	1		

- Molecule 22 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanadec-1-yl undecanoate (CCD ID: CN3) (formula: C₃₆H₆₈O₁₇P₂).



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

- Molecule 23 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 24 is water.

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

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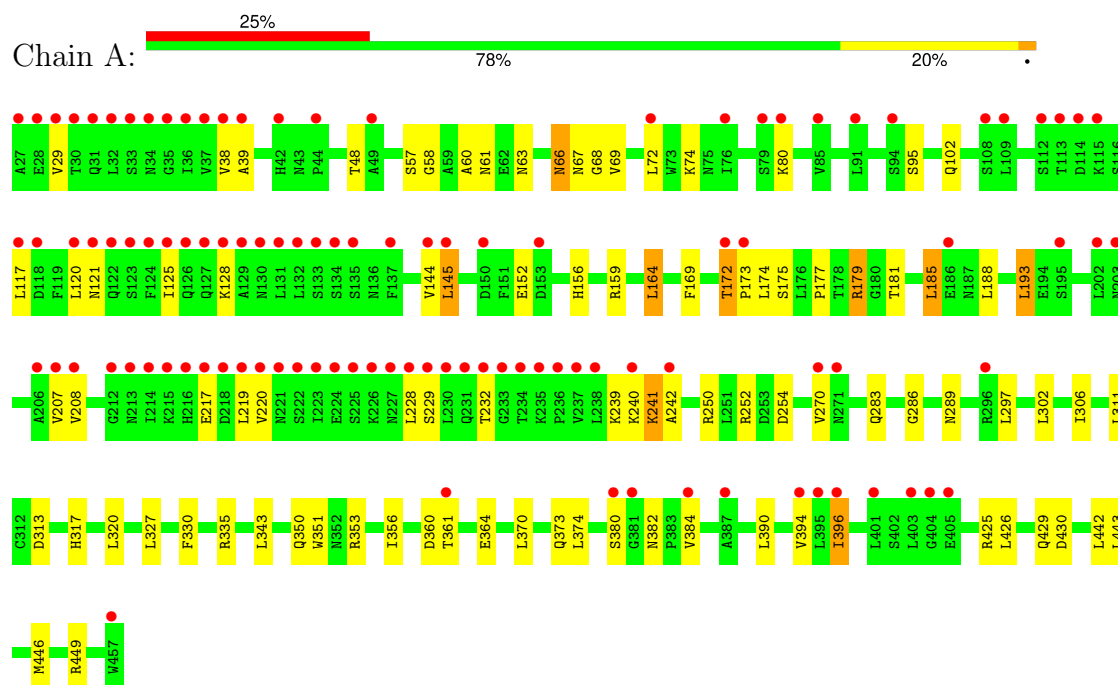
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	S	40	Total 40	O 40	0	0
24	T	12	Total 12	O 12	0	0
24	U	8	Total 8	O 8	0	0
24	V	2	Total 2	O 2	0	0
24	W	20	Total 20	O 20	0	0

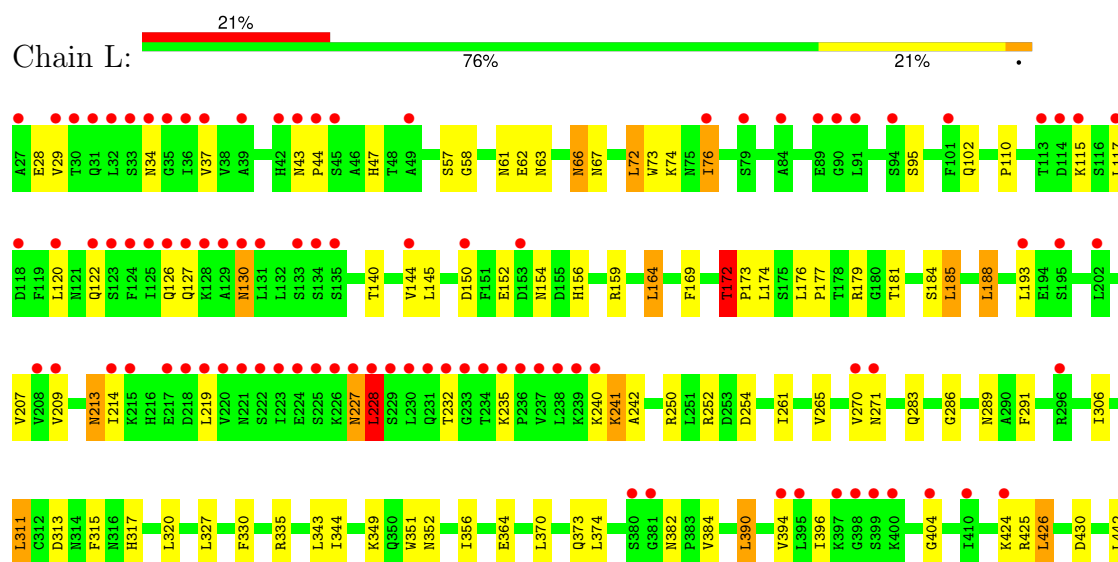
3 Residue-property plots

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

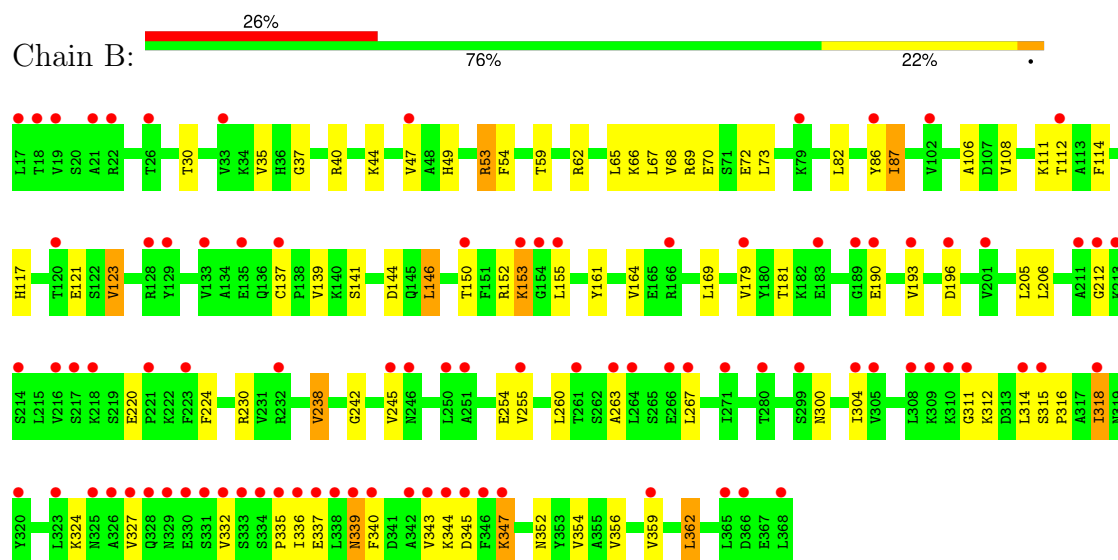


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

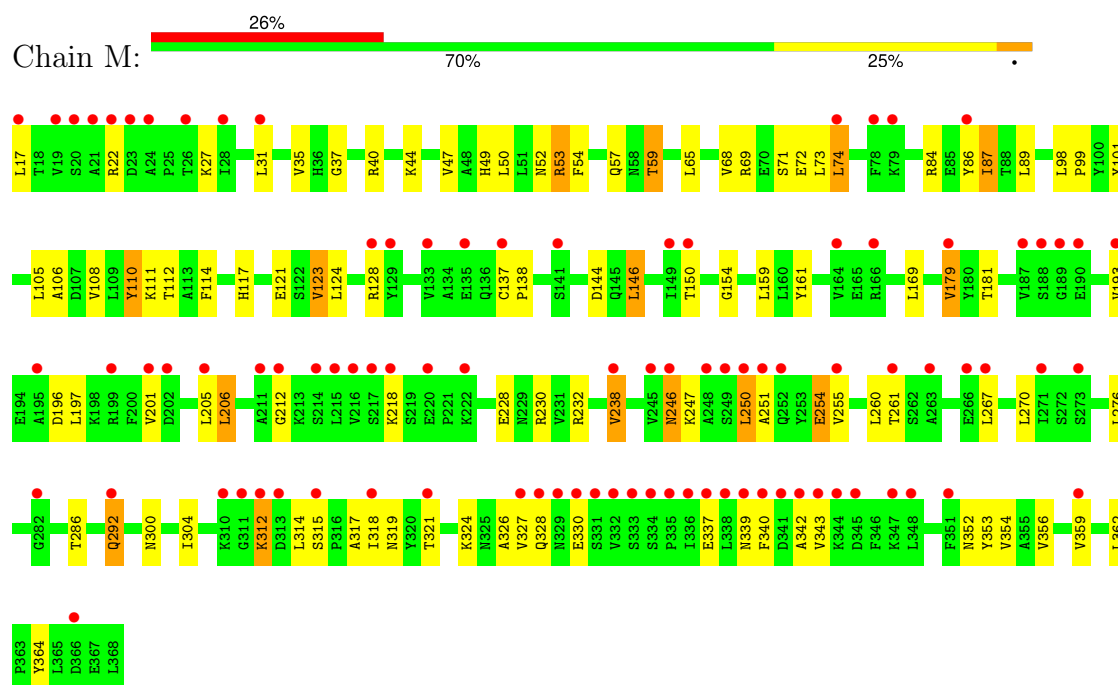




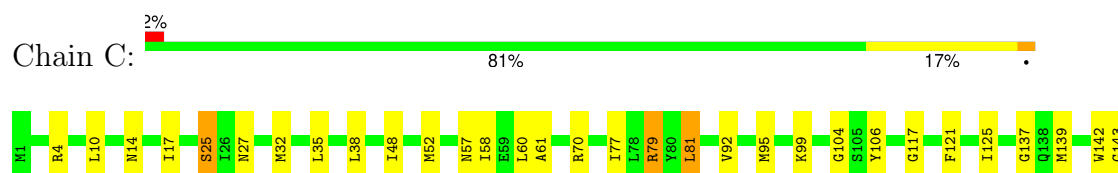
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

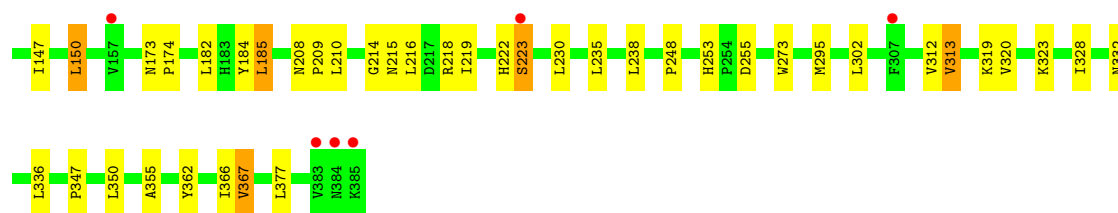


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

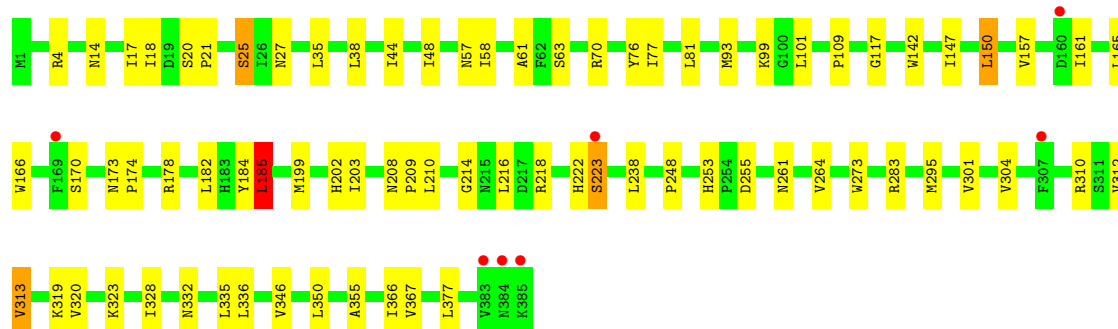
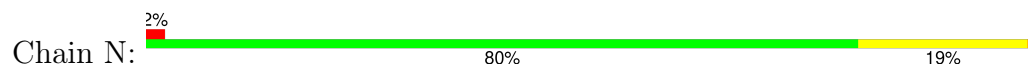


• Molecule 3: CYTOCHROME B

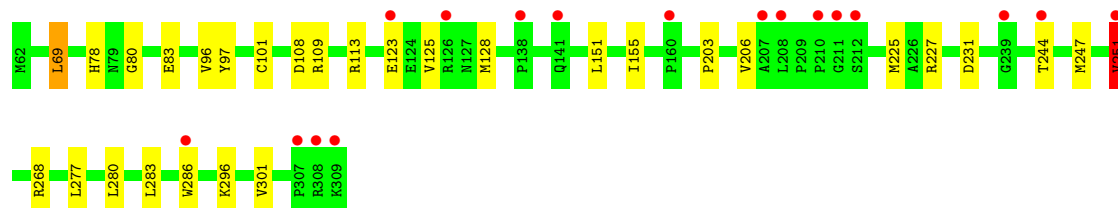
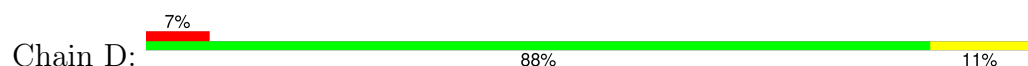




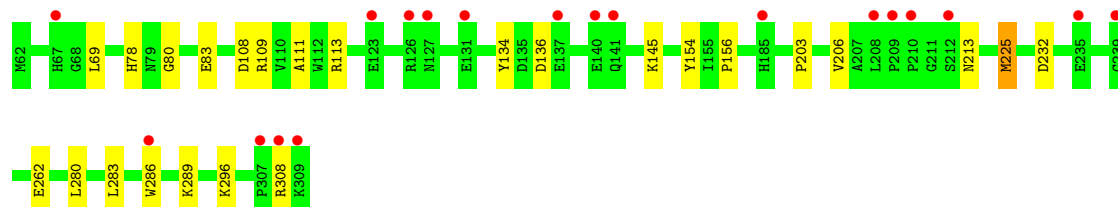
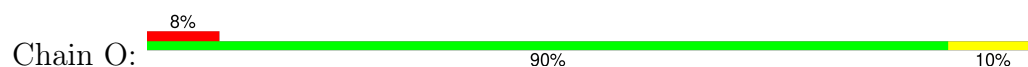
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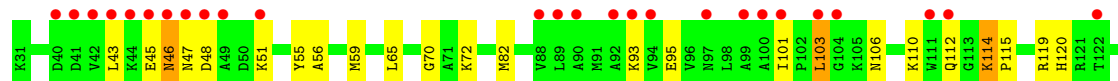
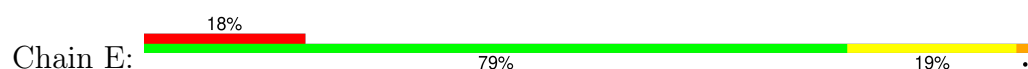
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



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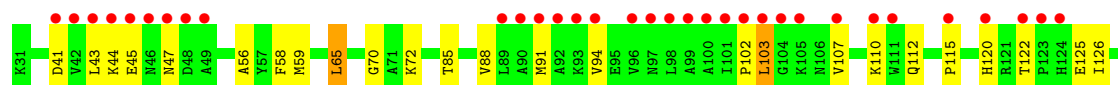
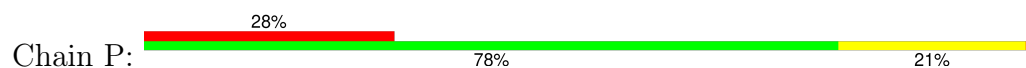


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

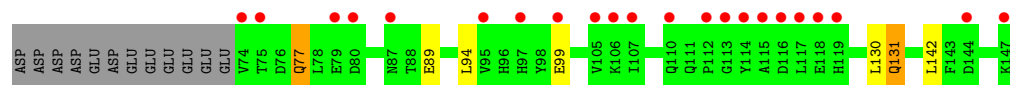




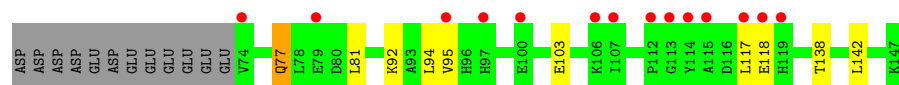
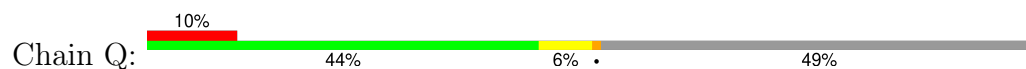
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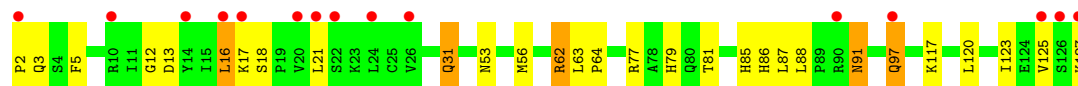
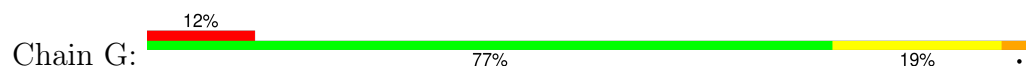
- Molecule 6: Cytochrome b-c1 complex subunit 6



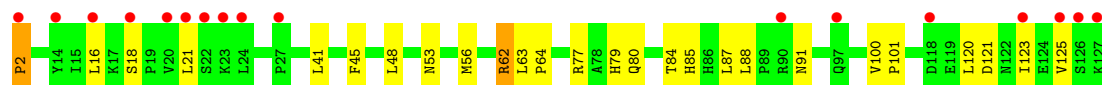
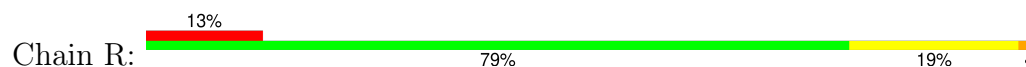
- Molecule 6: Cytochrome b-c1 complex subunit 6



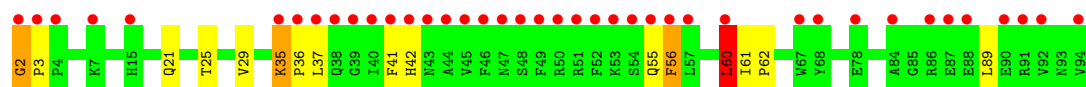
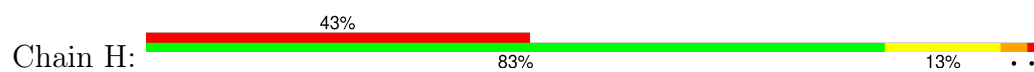
- Molecule 7: Cytochrome b-c1 complex subunit 7



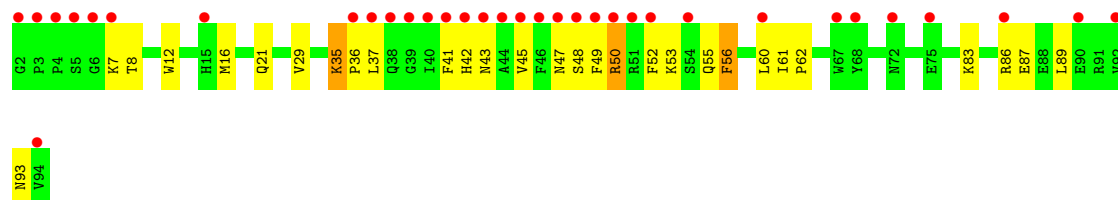
- Molecule 7: Cytochrome b-c1 complex subunit 7



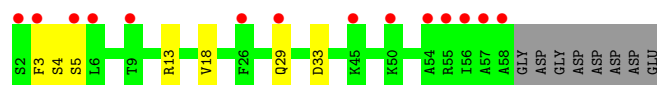
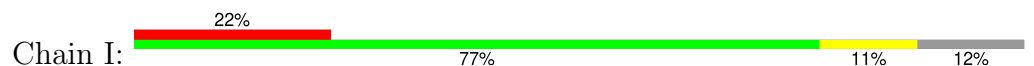
- Molecule 8: Cytochrome b-c1 complex subunit 8



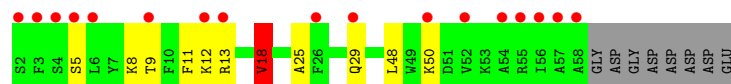
• Molecule 8: Cytochrome b-c1 complex subunit 8



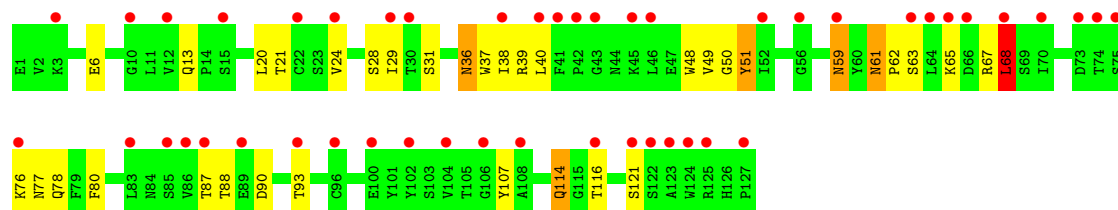
• Molecule 9: Cytochrome b-c1 complex subunit 9



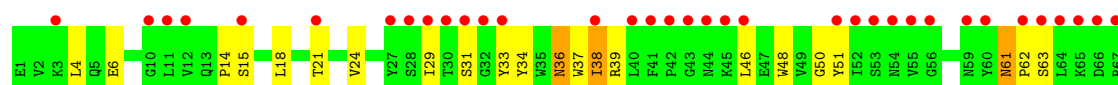
• Molecule 9: Cytochrome b-c1 complex subunit 9



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

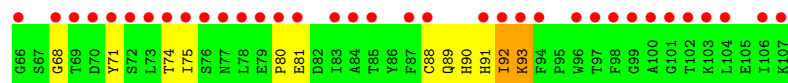
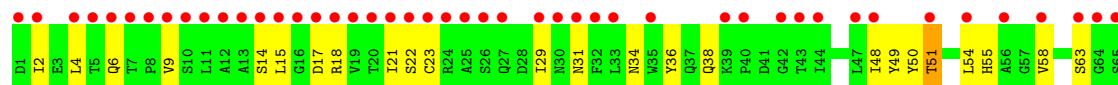
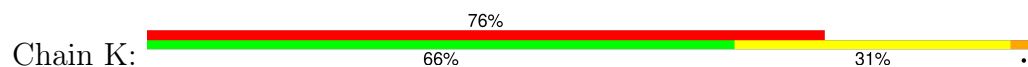


• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

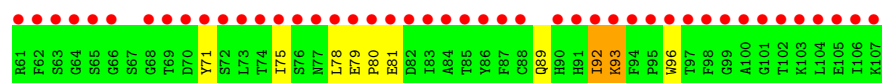
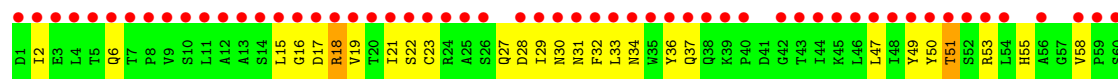




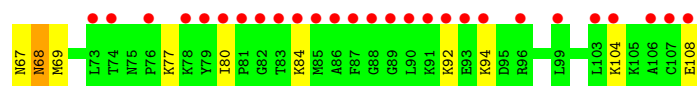
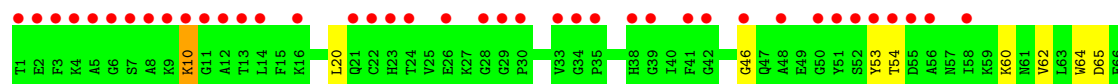
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT



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



• Molecule 12: Cytochrome c iso-1



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.12Å 165.09Å 194.37Å 90.00° 104.09° 90.00°	Depositor
Resolution (Å)	18.99 – 1.90 18.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (18.99-1.90) 95.1 (18.99-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.263 0.238 , 0.254	Depositor DCC
R_{free} test set	33007 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	38020	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

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

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: FES, CN3, 8PE, FRU, 6PH, GLC, CN5, 9PE, SMA, M3L, UMQ, HEM, 7PH

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	0.39	0/3405	0.91	6/4614 (0.1%)
1	L	0.39	0/3405	0.90	5/4614 (0.1%)
2	B	0.38	0/2781	0.92	9/3764 (0.2%)
2	M	0.38	0/2781	0.91	8/3764 (0.2%)
3	C	0.53	1/3192 (0.0%)	0.98	12/4354 (0.3%)
3	N	0.54	1/3192 (0.0%)	0.99	14/4354 (0.3%)
4	D	0.43	0/2022	0.95	8/2751 (0.3%)
4	O	0.47	1/2022 (0.0%)	0.96	5/2751 (0.2%)
5	E	0.44	0/1444	0.91	5/1957 (0.3%)
5	P	0.44	0/1444	0.93	5/1957 (0.3%)
6	F	0.36	0/638	0.82	1/858 (0.1%)
6	Q	0.38	0/638	0.82	1/858 (0.1%)
7	G	0.42	0/1040	0.89	2/1408 (0.1%)
7	R	0.46	0/1040	0.89	1/1408 (0.1%)
8	H	0.41	0/804	0.94	6/1088 (0.6%)
8	S	0.41	0/804	0.91	5/1088 (0.5%)
9	I	0.39	0/479	0.84	0/646
9	T	0.41	0/479	0.86	2/646 (0.3%)
10	J	0.36	0/1043	0.84	2/1422 (0.1%)
10	U	0.36	0/1043	0.88	4/1422 (0.3%)
11	K	0.36	0/863	0.72	0/1172
11	V	0.36	0/863	0.73	0/1172
12	W	0.36	0/865	0.89	2/1157 (0.2%)
All	All	0.43	3/36287 (0.0%)	0.91	103/49225 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	225	MET	SD-CE	-8.37	1.58	1.79
3	C	367	VAL	CA-CB	5.59	1.57	1.54
3	N	367	VAL	CA-CB	5.18	1.57	1.54

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	33	TYR	N-CA-C	8.39	116.81	108.75
8	H	2	GLY	CA-C-N	8.11	125.50	119.66
8	H	2	GLY	C-N-CA	8.11	125.50	119.66
5	P	163	GLY	N-CA-C	7.93	126.26	115.32
2	M	87	ILE	N-CA-C	-7.83	94.09	107.24
2	B	111	LYS	N-CA-C	7.79	121.20	110.06
4	O	108	ASP	N-CA-C	7.64	120.50	111.71
1	A	286	GLY	N-CA-C	7.42	124.33	111.78
2	B	87	ILE	N-CA-C	-7.37	94.86	107.24
2	M	111	LYS	N-CA-C	7.26	120.44	110.06
3	N	17	ILE	N-CA-C	7.17	120.08	113.20
6	Q	142	LEU	N-CA-C	6.87	119.35	111.11
6	F	142	LEU	N-CA-C	6.82	119.34	111.02
3	N	328	ILE	N-CA-C	-6.58	104.35	110.53
10	U	36	ASN	N-CA-C	6.57	120.19	110.46
4	O	83	GLU	N-CA-C	6.57	119.95	109.24
12	W	67	ASN	N-CA-C	6.49	118.15	111.14
10	J	36	ASN	N-CA-C	6.43	119.97	110.46
4	D	108	ASP	N-CA-C	6.42	120.68	112.34
4	D	251	VAL	CB-CA-C	-6.39	103.40	112.22
1	L	154	ASN	N-CA-C	6.33	121.89	114.04
3	C	185	LEU	N-CA-C	6.32	118.05	111.03
4	D	83	GLU	N-CA-C	6.29	119.49	109.24
3	N	70	ARG	N-CA-C	6.13	120.83	112.68
1	A	306	ILE	N-CA-C	6.05	121.36	113.07
5	E	163	GLY	N-CA-C	6.05	123.67	115.32
3	C	328	ILE	N-CA-C	-6.05	104.61	110.72
3	N	185	LEU	N-CA-C	6.03	117.65	111.14
3	C	70	ARG	N-CA-C	6.01	120.68	112.68
7	G	3	GLN	N-CA-C	-5.97	100.27	109.76
8	S	60	LEU	N-CA-C	5.97	117.79	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	286	GLY	N-CA-C	5.93	121.80	111.78
2	M	59	THR	N-CA-C	-5.91	101.45	110.14
8	S	50	ARG	N-CA-C	-5.90	104.43	111.69
8	S	56	PHE	N-CA-C	5.89	118.45	111.33
1	A	241	LYS	N-CA-C	5.87	118.78	110.50
5	P	139	ASP	CA-C-N	5.86	127.16	119.84
5	P	139	ASP	C-N-CA	5.86	127.16	119.84
3	C	273	TRP	N-CA-C	5.83	118.39	111.33
3	C	248	PRO	N-CA-C	5.79	121.10	113.86
2	M	179	VAL	N-CA-C	5.78	118.74	112.96
9	T	11	PHE	N-CA-C	5.77	122.27	113.61
10	J	68	LEU	N-CA-C	5.71	118.26	110.55
1	A	356	ILE	N-CA-C	5.69	121.18	109.34
3	N	248	PRO	N-CA-C	5.69	121.23	113.84
5	P	178	CYS	CA-C-N	5.66	125.28	119.56
5	P	178	CYS	C-N-CA	5.66	125.28	119.56
3	C	366	ILE	N-CA-C	5.66	115.85	110.42
2	B	86	TYR	N-CA-C	5.64	118.45	109.81
2	B	59	THR	N-CA-C	-5.64	101.85	110.14
1	L	356	ILE	N-CA-C	5.61	121.01	109.34
2	M	86	TYR	N-CA-C	5.61	118.39	109.81
2	M	110	TYR	N-CA-C	5.57	118.54	111.69
3	C	17	ILE	N-CA-C	5.55	118.97	113.53
2	B	123	VAL	N-CA-C	5.51	115.65	110.30
3	N	61	ALA	N-CA-C	5.49	117.72	111.02
3	C	219	ILE	N-CA-C	-5.47	104.70	109.19
8	H	56	PHE	N-CA-C	5.44	117.91	111.33
10	U	86	VAL	N-CA-C	5.42	116.33	110.21
7	R	87	LEU	N-CA-C	-5.41	101.75	110.14
8	H	60	LEU	N-CA-C	5.41	116.86	111.07
7	G	87	LEU	N-CA-C	-5.41	101.76	110.14
3	N	202	HIS	N-CA-C	5.40	117.17	111.28
8	S	35	LYS	CA-C-N	5.38	126.56	119.84
8	S	35	LYS	C-N-CA	5.38	126.56	119.84
3	N	273	TRP	N-CA-C	5.35	117.80	111.33
3	C	137	GLY	N-CA-C	-5.34	104.40	112.41
4	D	155	ILE	CA-C-N	5.31	125.21	119.85
4	D	155	ILE	C-N-CA	5.31	125.21	119.85
4	D	80	GLY	CA-C-N	5.30	125.11	119.28
4	D	80	GLY	C-N-CA	5.30	125.11	119.28
3	N	366	ILE	N-CA-C	5.29	115.50	110.42
8	H	35	LYS	CA-C-N	5.28	126.44	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	35	LYS	C-N-CA	5.28	126.44	119.84
3	C	25	SER	N-CA-C	5.26	119.80	113.17
2	B	318	ILE	N-CA-C	5.24	115.45	110.42
3	N	264	VAL	N-CA-C	5.22	115.49	107.77
3	C	61	ALA	N-CA-C	5.21	117.38	111.02
1	L	172	THR	CA-C-N	5.19	124.64	119.24
1	L	172	THR	C-N-CA	5.19	124.64	119.24
4	O	232	ASP	N-CA-C	5.18	119.18	112.86
2	M	57	GLN	N-CA-C	-5.17	101.72	109.79
3	C	215	ASN	N-CA-C	5.16	118.84	112.54
10	U	68	LEU	N-CA-C	5.16	117.19	110.53
5	E	180	CYS	N-CA-C	5.15	116.70	111.14
4	O	80	GLY	CA-C-N	5.15	125.44	119.47
4	O	80	GLY	C-N-CA	5.15	125.44	119.47
3	N	261	ASN	CA-C-N	5.14	124.86	119.82
3	N	261	ASN	C-N-CA	5.14	124.86	119.82
5	E	194	GLY	CA-C-N	5.13	124.74	119.56
5	E	194	GLY	C-N-CA	5.13	124.74	119.56
9	T	18	VAL	N-CA-C	5.13	115.75	110.36
2	B	220	GLU	CA-C-N	5.12	125.05	119.78
2	B	220	GLU	C-N-CA	5.12	125.05	119.78
1	A	396	ILE	N-CA-C	5.12	115.78	110.82
2	M	123	VAL	N-CA-C	5.12	115.26	110.30
1	A	446	MET	N-CA-C	5.08	116.82	111.28
2	B	153	LYS	N-CA-C	5.05	121.56	110.80
3	N	25	SER	N-CA-C	5.05	119.53	113.17
12	W	64	TRP	N-CA-C	5.05	117.48	109.96
5	E	101	ILE	N-CA-C	5.05	112.15	107.56
3	N	346	VAL	N-CA-C	-5.04	104.33	109.02
4	D	101	CYS	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	97	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3321	62	0
1	L	3344	0	3321	76	0
2	B	2735	0	2774	70	0
2	M	2735	0	2774	72	0
3	C	3090	0	3129	47	0
3	N	3090	0	3129	46	0
4	D	1961	0	1888	22	0
4	O	1961	0	1888	17	0
5	E	1411	0	1386	29	0
5	P	1411	0	1386	29	0
6	F	624	0	581	4	0
6	Q	624	0	581	6	0
7	G	1019	0	1034	22	0
7	R	1019	0	1034	19	0
8	H	773	0	736	10	0
8	S	773	0	736	20	0
9	I	465	0	459	7	0
9	T	465	0	459	9	0
10	J	1015	0	959	31	0
10	U	1015	0	959	27	0
11	K	842	0	820	28	0
11	V	842	0	820	28	0
12	W	859	0	862	14	0
13	X	23	0	21	5	0
14	A	40	0	59	1	0
14	L	40	0	59	3	0
15	A	34	0	44	2	0
15	L	34	0	44	2	0
16	C	86	0	60	2	0
16	D	43	0	30	1	0
16	N	86	0	60	4	0
16	O	43	0	30	0	0
16	W	43	0	30	0	0
17	C	37	0	42	2	0
17	N	37	0	42	1	0
18	C	47	0	73	1	0
18	N	47	0	73	0	0
19	C	40	0	59	0	0
19	N	40	0	59	0	0
20	C	41	0	50	5	0
21	D	38	0	55	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	O	38	0	55	2	0
22	D	55	0	66	5	0
22	N	55	0	66	5	0
23	E	4	0	0	0	0
23	P	4	0	0	0	0
24	A	153	0	0	2	0
24	B	93	0	0	8	0
24	C	161	0	0	2	0
24	D	154	0	0	5	0
24	E	74	0	0	0	0
24	F	16	0	0	0	0
24	G	71	0	0	1	0
24	H	31	0	0	0	0
24	I	11	0	0	0	0
24	J	15	0	0	0	0
24	K	7	0	0	0	0
24	L	170	0	0	0	0
24	M	101	0	0	1	0
24	N	170	0	0	1	0
24	O	173	0	0	7	0
24	P	66	0	0	2	0
24	Q	27	0	0	0	0
24	R	73	0	0	1	0
24	S	40	0	0	0	0
24	T	12	0	0	1	0
24	U	8	0	0	0	0
24	V	2	0	0	0	0
24	W	20	0	0	0	0
All	All	38020	0	36113	641	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (641) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:THR:HG22	2:B:352:ASN:HD22	1.27	1.00
2:M:246:ASN:HD22	2:M:246:ASN:H	1.11	0.99
6:F:77:GLN:H	6:F:77:GLN:HE21	1.12	0.97
2:M:150:THR:HG22	2:M:352:ASN:HD22	1.27	0.97
2:M:255:VAL:HG12	2:M:321:THR:HG21	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:ASN:H	1:L:66:ASN:HD21	1.10	0.92
1:A:63:ASN:H	1:A:66:ASN:HD21	1.18	0.91
3:C:52:MET:HE1	5:E:82:MET:HG2	1.52	0.91
10:J:114:GLN:H	10:J:114:GLN:HE21	1.21	0.88
3:C:32:MET:HE3	3:C:92:VAL:HG13	1.56	0.88
7:R:77:ARG:HD3	7:R:88:LEU:HD11	1.56	0.88
10:J:29:ILE:H	10:J:77:ASN:HD21	1.16	0.87
6:Q:77:GLN:H	6:Q:77:GLN:HE21	1.14	0.86
12:W:20:LEU:HD23	13:X:2:FRU:H12	1.58	0.86
2:B:318:ILE:HD11	2:B:340:PHE:HB3	1.59	0.84
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.60	0.84
11:K:31:ASN:HD22	11:K:51:THR:HG21	1.42	0.83
22:N:4131:CN3:HAA	7:R:85:HIS:NE2	1.93	0.83
2:B:150:THR:HG22	2:B:352:ASN:ND2	1.92	0.83
2:M:150:THR:HG22	2:M:352:ASN:ND2	1.92	0.83
1:A:361:THR:HG21	7:R:123:ILE:O	1.80	0.82
12:W:60:LYS:HG3	12:W:62:VAL:HG23	1.62	0.82
1:A:63:ASN:H	1:A:66:ASN:ND2	1.78	0.82
2:B:49:HIS:HD2	2:B:161:TYR:H	1.28	0.81
1:L:317:HIS:HE1	1:L:351:TRP:HE1	1.28	0.80
1:A:179:ARG:HH21	1:A:179:ARG:HG2	1.47	0.80
2:M:246:ASN:H	2:M:246:ASN:ND2	1.80	0.79
2:M:318:ILE:HD11	2:M:340:PHE:HB3	1.65	0.79
6:Q:77:GLN:H	6:Q:77:GLN:NE2	1.81	0.78
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.30	0.77
2:M:49:HIS:HD2	2:M:161:TYR:H	1.33	0.77
3:N:58:ILE:H	3:N:173:ASN:HD22	1.29	0.77
10:U:29:ILE:H	10:U:77:ASN:HD21	1.32	0.77
1:L:63:ASN:H	1:L:66:ASN:ND2	1.82	0.77
7:G:31:GLN:HA	7:G:31:GLN:HE21	1.50	0.77
6:F:77:GLN:H	6:F:77:GLN:NE2	1.82	0.76
1:A:58:GLY:H	1:A:61:ASN:HD22	1.32	0.76
22:D:4031:CN3:HAA	7:G:85:HIS:NE2	2.02	0.75
3:N:214:GLY:O	3:N:218:ARG:HD2	1.87	0.75
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.69	0.75
2:B:108:VAL:O	2:B:112:THR:HG23	1.86	0.75
2:B:238:VAL:HG13	2:B:356:VAL:HB	1.68	0.74
2:M:37:GLY:HA3	2:M:179:VAL:HG11	1.68	0.74
10:J:6:GLU:H	10:J:114:GLN:HE22	1.35	0.74
5:P:172:ASP:H	5:P:184:HIS:HD2	1.36	0.74
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:95:GLU:HG2	5:E:213:ILE:HG22	1.70	0.73
10:U:114:GLN:H	10:U:114:GLN:HE21	1.35	0.73
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.54	0.72
2:M:108:VAL:O	2:M:112:THR:HG23	1.87	0.72
3:C:58:ILE:H	3:C:173:ASN:HD22	1.36	0.72
4:O:225:MET:HE2	24:O:5654:HOH:O	1.90	0.71
2:B:62:ARG:HG2	2:B:62:ARG:HH21	1.54	0.71
7:R:77:ARG:HD2	24:R:5803:HOH:O	1.91	0.70
3:N:253:HIS:HD2	3:N:255:ASP:H	1.38	0.70
5:P:115:PRO:HD2	5:P:158:ILE:HD11	1.73	0.70
11:K:6:GLN:HG2	11:K:23:CYS:SG	2.31	0.70
1:L:404:GLY:HA2	2:M:27:LYS:HE3	1.72	0.70
1:L:179:ARG:HG2	1:L:179:ARG:HH21	1.55	0.70
1:L:283:GLN:NE2	1:L:373:GLN:HE21	1.90	0.70
2:M:324:LYS:O	2:M:327:VAL:HG22	1.93	0.69
2:B:260:LEU:HD22	2:B:267:LEU:HD11	1.72	0.69
7:G:125:VAL:HG21	1:L:364:GLU:HG3	1.73	0.69
3:C:312:VAL:HG21	7:G:5:PHE:CE1	2.28	0.68
3:C:253:HIS:HD2	3:C:255:ASP:H	1.41	0.68
3:N:323:LYS:NZ	8:S:55:GLN:HE22	1.91	0.68
2:B:62:ARG:NH2	2:B:67:LEU:HD13	2.08	0.67
11:V:2:ILE:HD12	11:V:2:ILE:H	1.59	0.67
2:M:238:VAL:HG13	2:M:356:VAL:HB	1.75	0.67
5:P:172:ASP:H	5:P:184:HIS:CD2	2.11	0.67
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.42	0.67
2:B:300:ASN:O	2:B:304:ILE:HG12	1.95	0.66
2:M:300:ASN:O	2:M:304:ILE:HG12	1.95	0.66
4:D:227:ARG:HH11	4:D:244:THR:HG21	1.59	0.66
2:M:260:LEU:HD22	2:M:267:LEU:HD11	1.78	0.66
1:L:117:LEU:HD11	1:L:219:LEU:HD12	1.76	0.66
3:N:44:ILE:O	3:N:48:ILE:HG12	1.94	0.66
1:L:317:HIS:CE1	1:L:351:TRP:HE1	2.13	0.66
12:W:65:ASP:H	12:W:68:ASN:HD21	1.44	0.66
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.13	0.65
1:A:382:ASN:OD1	1:A:384:VAL:HG22	1.96	0.65
11:V:36:TYR:HE2	11:V:89:GLN:HG2	1.60	0.65
20:C:4033:CN5:H3CA	14:L:4113:6PH:H2E	1.79	0.65
1:L:58:GLY:H	1:L:61:ASN:HD22	1.45	0.65
1:L:207:VAL:HG11	1:L:394:VAL:HG21	1.80	0.64
2:B:49:HIS:CD2	2:B:161:TYR:H	2.14	0.64
2:M:31:LEU:HD12	2:M:105:LEU:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:320:VAL:HG23	24:C:7051:HOH:O	1.97	0.64
2:B:137:CYS:SG	24:B:8522:HOH:O	2.55	0.64
1:L:122:GLN:HA	1:L:126:GLN:HB3	1.79	0.63
2:M:247:LYS:O	2:M:250:LEU:HD22	1.98	0.63
1:L:72:LEU:HD23	1:L:193:LEU:HD21	1.80	0.63
5:P:91:MET:HG2	5:P:112:GLN:NE2	2.14	0.63
1:L:72:LEU:HB3	1:L:193:LEU:HD11	1.79	0.63
10:U:21:THR:HG22	10:U:80:PHE:HD2	1.63	0.63
1:A:68:GLY:HA3	1:A:185:LEU:HD11	1.81	0.63
2:B:164:VAL:HG21	2:M:232:ARG:HH11	1.63	0.62
1:L:72:LEU:HD22	1:L:188:LEU:HD23	1.79	0.62
4:O:213:ASN:OD1	13:X:2:FRU:H62	1.99	0.62
4:D:113:ARG:HG2	4:D:151:LEU:O	1.99	0.62
5:P:134:MET:HG3	10:U:31:SER:HB3	1.81	0.62
5:E:48:ASP:HB3	5:E:51:LYS:HG2	1.80	0.62
5:E:172:ASP:H	5:E:184:HIS:HD2	1.47	0.62
3:C:208:ASN:HD22	3:C:210:LEU:H	1.47	0.62
4:O:113:ARG:NE	24:O:6841:HOH:O	2.27	0.62
2:B:146:LEU:O	2:B:150:THR:HG23	2.00	0.62
20:C:4033:CN5:H3E	14:L:4113:6PH:H2B	1.82	0.62
2:M:65:LEU:O	2:M:69:ARG:HG2	1.99	0.62
10:U:6:GLU:H	10:U:114:GLN:HE22	1.48	0.62
1:A:121:ASN:ND2	1:A:125:ILE:HD12	2.14	0.61
7:G:77:ARG:HD2	24:G:5303:HOH:O	1.99	0.61
2:B:336:ILE:HD12	2:B:336:ILE:H	1.64	0.61
3:C:27:ASN:HB2	22:D:4031:CN3:O2'	1.99	0.61
1:A:117:LEU:HD11	1:A:219:LEU:HD12	1.83	0.61
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.82	0.61
9:T:5:SER:O	9:T:9:THR:HG23	2.01	0.61
3:N:208:ASN:HD22	3:N:210:LEU:H	1.49	0.60
3:N:253:HIS:CD2	3:N:255:ASP:H	2.17	0.60
3:N:320:VAL:HG23	24:N:6971:HOH:O	2.02	0.60
10:U:29:ILE:HG12	10:U:77:ASN:ND2	2.16	0.60
10:J:28:SER:HB3	10:J:31:SER:OG	2.02	0.60
12:W:54:THR:CG2	12:W:84:LYS:HG3	2.31	0.60
1:A:72:LEU:HD23	1:A:193:LEU:HD21	1.83	0.60
2:M:71:SER:HA	2:M:74:LEU:CD1	2.32	0.59
3:N:58:ILE:H	3:N:173:ASN:ND2	1.99	0.59
9:T:8:LYS:O	9:T:12:LYS:HD2	2.02	0.59
3:C:4:ARG:HE	3:C:14:ASN:ND2	2.00	0.59
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:29:ILE:HG12	10:J:77:ASN:ND2	2.18	0.59
12:W:20:LEU:HD23	13:X:2:FRU:C1	2.31	0.59
3:N:27:ASN:HB2	22:N:4131:CN3:O2'	2.02	0.59
11:V:79:GLU:HB3	11:V:80:PRO:HD3	1.84	0.59
2:B:193:VAL:HG23	2:B:196:ASP:HB2	1.85	0.59
1:L:72:LEU:CD1	1:L:144:VAL:HG21	2.33	0.59
1:A:179:ARG:HG2	1:A:179:ARG:NH2	2.14	0.59
2:B:30:THR:CG2	2:B:190:GLU:HB3	2.33	0.59
1:L:252:ARG:HD3	1:L:254:ASP:OD1	2.03	0.59
4:D:227:ARG:NH1	4:D:244:THR:HG21	2.18	0.58
10:J:24:VAL:HG21	10:J:29:ILE:HD11	1.85	0.58
10:J:29:ILE:H	10:J:77:ASN:ND2	1.94	0.58
8:S:83:LYS:O	8:S:86:ARG:HG2	2.04	0.58
1:L:241:LYS:H	1:L:241:LYS:HD2	1.68	0.58
1:A:217:GLU:HA	1:A:220:VAL:HG12	1.86	0.58
1:A:228:LEU:HG	1:A:229:SER:H	1.67	0.58
2:B:121:GLU:OE2	7:R:62:ARG:HD2	2.04	0.58
8:H:56:PHE:O	8:H:60:LEU:HB2	2.03	0.58
1:L:156:HIS:HD2	1:L:159:ARG:HH21	1.51	0.58
3:C:253:HIS:CD2	3:C:255:ASP:H	2.21	0.58
1:A:283:GLN:HE22	1:A:373:GLN:HE21	1.52	0.58
3:C:214:GLY:O	3:C:218:ARG:HD2	2.03	0.58
6:F:77:GLN:HE21	6:F:77:GLN:N	1.93	0.58
4:D:247:MET:O	4:D:251:VAL:HG22	2.05	0.57
11:K:36:TYR:CE2	11:K:89:GLN:HG2	2.37	0.57
1:A:429:GLN:HE22	9:I:13:ARG:HH21	1.50	0.57
7:G:97:GLN:H	7:G:97:GLN:NE2	2.03	0.57
1:L:289:ASN:C	1:L:289:ASN:HD22	2.12	0.57
2:M:181:THR:HB	2:M:212:GLY:H	1.70	0.57
2:B:315:SER:OG	2:B:344:LYS:HD2	2.04	0.57
7:G:53:ASN:ND2	7:G:56:MET:H	2.03	0.57
7:G:63:LEU:HD12	7:G:64:PRO:HD2	1.87	0.56
7:G:91:ASN:H	7:G:91:ASN:ND2	2.02	0.56
1:A:283:GLN:NE2	1:A:373:GLN:HE21	2.03	0.56
2:B:117:HIS:HB3	7:R:62:ARG:HG2	1.88	0.56
10:J:114:GLN:H	10:J:114:GLN:NE2	1.96	0.56
1:L:110:PRO:HB3	1:L:213:ASN:HB3	1.87	0.56
2:M:49:HIS:CD2	2:M:161:TYR:H	2.20	0.56
2:B:347:LYS:HD3	2:B:347:LYS:N	2.20	0.56
2:M:110:TYR:CD2	2:M:205:LEU:HD23	2.41	0.56
2:M:35:VAL:CG1	2:M:179:VAL:HG12	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:VAL:CG2	2:M:232:ARG:HH11	2.18	0.56
5:P:103:LEU:O	5:P:120:HIS:HB3	2.06	0.56
3:N:313:VAL:HG22	3:N:319:LYS:HE3	1.87	0.56
2:B:53:ARG:HB3	2:B:123:VAL:HG13	1.89	0.55
10:U:61:ASN:HD22	10:U:63:SER:H	1.52	0.55
2:B:30:THR:HG22	2:B:190:GLU:HB3	1.87	0.55
3:C:313:VAL:HG22	3:C:319:LYS:HE3	1.88	0.55
1:L:270:VAL:O	1:L:271:ASN:HB2	2.05	0.55
15:A:4021:UMQ:HC1	9:I:18:VAL:HG12	1.88	0.55
1:A:58:GLY:H	1:A:61:ASN:ND2	2.02	0.55
4:D:125:VAL:HA	4:D:128:MET:HE3	1.89	0.55
22:D:4031:CN3:HAA	7:G:85:HIS:CE1	2.41	0.55
10:J:20:LEU:HD22	10:J:116:THR:HG21	1.89	0.55
10:J:65:LYS:HA	10:J:68:LEU:HD11	1.87	0.55
3:N:4:ARG:HE	3:N:14:ASN:ND2	2.04	0.55
10:U:29:ILE:H	10:U:77:ASN:ND2	2.02	0.55
5:E:172:ASP:H	5:E:184:HIS:CD2	2.25	0.55
5:P:72:LYS:NZ	9:T:29:GLN:HE22	2.04	0.55
12:W:20:LEU:CD2	13:X:2:FRU:H12	2.34	0.55
11:V:29:ILE:HG22	11:V:92:ILE:HD12	1.88	0.55
2:M:193:VAL:HG23	2:M:196:ASP:HB2	1.88	0.55
3:N:57:ASN:HA	3:N:173:ASN:HD21	1.71	0.55
5:P:103:LEU:HG	5:P:122:THR:HG22	1.88	0.55
10:U:61:ASN:HD22	10:U:61:ASN:C	2.15	0.55
5:E:51:LYS:HD3	9:I:4:SER:HB2	1.88	0.54
5:P:91:MET:HG2	5:P:112:GLN:HE21	1.70	0.54
3:N:323:LYS:CE	8:S:55:GLN:HE22	2.21	0.54
7:R:53:ASN:ND2	7:R:56:MET:H	2.05	0.54
1:L:169:PHE:O	1:L:172:THR:HB	2.08	0.54
11:V:37:GLN:HB2	11:V:47:LEU:HD11	1.89	0.54
10:J:21:THR:HG22	10:J:80:PHE:HD2	1.73	0.54
10:J:61:ASN:C	10:J:61:ASN:HD22	2.16	0.54
11:K:55:HIS:O	11:K:58:VAL:HG22	2.08	0.54
6:Q:81:LEU:HB3	6:Q:138:THR:HG22	1.89	0.54
2:B:44:LYS:O	2:B:47:VAL:HG23	2.07	0.54
3:C:52:MET:HE3	3:N:178:ARG:HB2	1.89	0.54
3:N:147:ILE:HA	3:N:150:LEU:HD22	1.90	0.54
2:B:336:ILE:HG21	2:B:339:ASN:HD22	1.73	0.54
3:N:208:ASN:HB2	3:N:209:PRO:HD2	1.91	0.53
5:P:58:PHE:HD2	5:P:59:MET:HE2	1.73	0.53
3:C:58:ILE:H	3:C:173:ASN:ND2	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:67:ASN:HD21	1:L:177:PRO:HG2	1.74	0.53
1:L:179:ARG:HG2	1:L:179:ARG:NH2	2.23	0.53
11:V:55:HIS:O	11:V:58:VAL:HG22	2.09	0.53
1:A:164:LEU:HD13	1:A:327:LEU:HD13	1.91	0.53
1:L:313:ASP:OD1	1:L:335:ARG:HD3	2.09	0.53
5:E:213:ILE:O	5:E:213:ILE:HG13	2.08	0.53
7:R:63:LEU:HD12	7:R:64:PRO:HD2	1.91	0.53
7:G:62:ARG:HD2	2:M:121:GLU:OE2	2.08	0.53
2:M:71:SER:HA	2:M:74:LEU:HD11	1.89	0.53
8:S:89:LEU:O	8:S:93:ASN:HB2	2.08	0.53
1:A:207:VAL:HG11	1:A:394:VAL:HG21	1.90	0.53
1:L:382:ASN:OD1	1:L:384:VAL:HG22	2.08	0.53
1:A:302:LEU:HB2	1:A:350:GLN:HG3	1.91	0.53
2:M:53:ARG:HB3	2:M:123:VAL:HG13	1.89	0.53
10:U:14:PRO:O	10:U:15:SER:HB3	2.09	0.53
1:L:130:ASN:H	1:L:130:ASN:HD22	1.57	0.53
2:M:251:ALA:HB2	2:M:339:ASN:HB2	1.91	0.53
2:M:255:VAL:HG11	2:M:343:VAL:HG21	1.91	0.53
4:O:286:TRP:CE3	5:P:59:MET:HG3	2.44	0.53
12:W:104:LYS:O	12:W:108:GLU:HG2	2.08	0.53
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.90	0.53
2:M:255:VAL:HG23	2:M:314:LEU:HD13	1.91	0.53
2:M:292:GLN:H	2:M:292:GLN:NE2	2.06	0.53
2:B:238:VAL:CG1	2:B:356:VAL:HB	2.36	0.52
2:M:246:ASN:ND2	2:M:246:ASN:N	2.52	0.52
3:N:184:TYR:CD1	16:N:4021:HEM:HBC1	2.44	0.52
8:S:61:ILE:HB	8:S:62:PRO:HD3	1.91	0.52
10:U:87:THR:HG22	10:U:88:THR:N	2.24	0.52
1:A:289:ASN:C	1:A:289:ASN:HD22	2.16	0.52
10:U:61:ASN:ND2	10:U:63:SER:H	2.06	0.52
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.90	0.52
2:M:146:LEU:O	2:M:150:THR:HG23	2.09	0.52
2:B:65:LEU:HD11	2:B:69:ARG:NH2	2.23	0.52
1:L:306:ILE:HA	1:L:311:LEU:HD22	1.92	0.52
1:A:350:GLN:HE22	1:A:353:ARG:HH21	1.57	0.52
2:B:35:VAL:CG1	2:B:179:VAL:HG12	2.39	0.52
2:M:238:VAL:CG1	2:M:356:VAL:HB	2.39	0.52
11:V:34:ASN:HD22	11:V:49:TYR:HA	1.75	0.52
2:B:311:GLY:O	2:B:312:LYS:HD2	2.09	0.52
7:G:81:THR:HG22	7:G:86:HIS:O	2.10	0.52
4:O:78:HIS:HD2	24:O:5586:HOH:O	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:77:GLN:HE21	6:Q:77:GLN:N	1.94	0.52
1:L:66:ASN:HA	1:L:188:LEU:HD11	1.90	0.52
2:M:106:ALA:HA	2:M:206:LEU:HD13	1.92	0.52
1:L:76:ILE:HG23	1:L:140:THR:HG21	1.92	0.52
1:L:344:ILE:HG21	1:L:448:ILE:HD12	1.91	0.52
2:M:68:VAL:O	2:M:72:GLU:HG3	2.10	0.52
5:P:72:LYS:HZ3	9:T:29:GLN:HE22	1.57	0.52
7:G:117:LYS:HE2	24:M:7272:HOH:O	2.09	0.52
2:M:146:LEU:HD23	2:M:286:THR:HG22	1.91	0.52
11:K:15:LEU:HD12	11:K:15:LEU:H	1.75	0.52
1:L:28:GLU:HG2	1:L:29:VAL:N	2.25	0.52
2:M:31:LEU:HD12	2:M:105:LEU:CD1	2.40	0.52
1:A:145:LEU:CD1	1:A:185:LEU:HB3	2.40	0.51
3:C:4:ARG:HE	3:C:14:ASN:HD21	1.56	0.51
3:C:147:ILE:O	3:C:150:LEU:HB2	2.09	0.51
10:J:51:TYR:C	10:J:51:TYR:CD2	2.89	0.51
12:W:68:ASN:HD22	12:W:69:MET:N	2.08	0.51
4:D:286:TRP:CZ3	5:E:56:ALA:HA	2.45	0.51
1:L:181:THR:O	1:L:185:LEU:HB2	2.09	0.51
6:Q:117:LEU:O	6:Q:118:GLU:HG2	2.09	0.51
10:U:4:LEU:HG	10:U:24:VAL:HG22	1.91	0.51
21:D:4014:7PH:H35	5:E:70:GLY:HA3	1.93	0.51
7:G:13:ASP:HB3	7:G:17:LYS:HE3	1.93	0.51
3:N:310:ARG:HA	7:R:2:PRO:HB2	1.92	0.51
1:L:172:THR:CG2	1:L:242:ALA:HA	2.41	0.51
3:N:63:SER:OG	4:O:109:ARG:NH1	2.43	0.51
7:G:91:ASN:H	7:G:91:ASN:HD22	1.58	0.51
1:L:28:GLU:HG2	1:L:29:VAL:H	1.74	0.51
10:J:114:GLN:HE21	10:J:114:GLN:N	2.00	0.51
1:L:283:GLN:HE21	1:L:373:GLN:HE21	1.58	0.51
4:D:231:ASP:OD1	4:D:244:THR:HG23	2.10	0.51
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.44	0.50
4:D:225:MET:HB2	16:D:4003:HEM:C1D	2.46	0.50
8:S:52:PHE:O	8:S:56:PHE:HB3	2.12	0.50
3:C:52:MET:CE	5:E:82:MET:HG2	2.32	0.50
20:C:4033:CN5:HB	20:C:4033:CN5:H1'A	1.92	0.50
2:M:261:THR:O	2:M:261:THR:HG22	2.11	0.50
1:A:313:ASP:OD1	1:A:335:ARG:HD3	2.12	0.50
7:G:62:ARG:HG2	2:M:117:HIS:HB3	1.92	0.50
1:L:67:ASN:HD22	1:L:181:THR:HG23	1.76	0.50
5:P:122:THR:O	5:P:126:ILE:HG13	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:240:LYS:HG2	1:L:241:LYS:N	2.26	0.50
4:O:289:LYS:HB2	8:S:37:LEU:HD13	1.92	0.50
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.42	0.50
10:U:38:ILE:HD12	10:U:46:LEU:HD22	1.92	0.50
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.12	0.50
3:C:79:ARG:NH1	24:C:6790:HOH:O	2.45	0.50
15:L:4121:UMQ:O1'	9:T:18:VAL:HG13	2.11	0.50
2:B:112:THR:HG22	24:B:6011:HOH:O	2.12	0.50
3:C:235:LEU:HD23	22:D:4031:CN3:H45	1.93	0.50
5:E:103:LEU:O	5:E:120:HIS:HB3	2.12	0.50
11:K:29:ILE:HD11	11:K:71:TYR:CE1	2.47	0.50
1:A:67:ASN:HD21	1:A:177:PRO:HG2	1.75	0.50
10:U:114:GLN:H	10:U:114:GLN:NE2	2.07	0.50
7:G:12:GLY:O	7:G:16:LEU:HD22	2.11	0.49
22:N:4131:CN3:HC	24:O:6998:HOH:O	2.12	0.49
1:L:241:LYS:H	1:L:241:LYS:CD	2.25	0.49
1:L:265:VAL:HG21	1:L:426:LEU:HD12	1.93	0.49
3:N:222:HIS:O	3:N:223:SER:HB2	2.10	0.49
21:O:4114:7PH:H35	5:P:70:GLY:HA3	1.94	0.49
8:S:42:HIS:H	8:S:45:VAL:HG12	1.76	0.49
2:B:146:LEU:HD13	2:B:354:VAL:HG22	1.94	0.49
11:K:2:ILE:HD11	11:K:93:LYS:NZ	2.28	0.49
3:C:295:MET:SD	17:C:4005:SMA:H1	2.52	0.49
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.47	0.49
1:L:172:THR:HG23	1:L:242:ALA:HA	1.95	0.49
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.47	0.49
15:L:4121:UMQ:HC1	9:T:18:VAL:HG12	1.94	0.49
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.77	0.49
2:M:260:LEU:CD2	2:M:267:LEU:HD11	2.42	0.49
3:N:4:ARG:HE	3:N:14:ASN:HD21	1.58	0.49
3:N:147:ILE:O	3:N:150:LEU:HB2	2.13	0.49
11:K:2:ILE:HD12	11:K:2:ILE:N	2.27	0.49
1:A:297:LEU:O	2:B:69:ARG:NH2	2.40	0.49
1:L:270:VAL:HG21	1:L:396:ILE:HD13	1.94	0.49
1:A:229:SER:HB3	1:A:232:THR:HB	1.95	0.49
1:A:48:THR:HG21	2:B:327:VAL:HG12	1.95	0.48
4:D:109:ARG:NH2	24:D:6205:HOH:O	2.46	0.48
10:J:37:TRP:O	10:J:49:VAL:HB	2.13	0.48
11:K:31:ASN:ND2	11:K:51:THR:HG21	2.21	0.48
11:K:34:ASN:HD22	11:K:49:TYR:HA	1.76	0.48
4:D:78:HIS:HD2	24:D:5086:HOH:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:2:ILE:HD12	11:K:2:ILE:H	1.78	0.48
3:N:218:ARG:HG3	8:S:16:MET:HE3	1.94	0.48
4:O:203:PRO:HG2	4:O:206:VAL:HG21	1.94	0.48
1:A:68:GLY:HA3	1:A:185:LEU:CD1	2.42	0.48
3:C:222:HIS:O	3:C:223:SER:HB2	2.12	0.48
11:V:17:ASP:O	11:V:78:LEU:HD13	2.14	0.48
11:V:53:ARG:HH21	11:V:53:ARG:HG3	1.77	0.48
1:A:250:ARG:NH1	1:A:442:LEU:O	2.47	0.48
11:V:47:LEU:HA	11:V:58:VAL:HG11	1.96	0.48
12:W:92:LYS:HD2	12:W:94:LYS:HE2	1.95	0.48
7:R:120:LEU:HA	7:R:123:ILE:HG23	1.94	0.48
12:W:60:LYS:HG2	12:W:80:ILE:HG12	1.94	0.48
5:E:93:LYS:HD3	5:E:215:GLY:HA3	1.95	0.48
10:J:29:ILE:N	10:J:77:ASN:HD21	1.98	0.48
2:M:292:GLN:H	2:M:292:GLN:CD	2.22	0.48
11:V:19:VAL:HG12	11:V:75:ILE:HB	1.96	0.48
2:B:318:ILE:HG22	24:B:8526:HOH:O	2.12	0.48
2:B:318:ILE:CD1	2:B:340:PHE:HB3	2.39	0.48
11:K:18:ARG:HB2	11:K:75:ILE:O	2.14	0.48
1:L:250:ARG:NH1	1:L:442:LEU:O	2.47	0.48
5:P:125:GLU:HB3	5:P:187:ILE:HG12	1.95	0.48
1:A:252:ARG:HD2	8:H:21:GLN:HB2	1.94	0.47
4:D:123:GLU:CD	4:D:123:GLU:H	2.21	0.47
5:P:65:LEU:HD13	9:T:25:ALA:HA	1.96	0.47
5:P:214:VAL:N	24:P:7409:HOH:O	2.46	0.47
1:L:66:ASN:H	1:L:66:ASN:HD22	1.63	0.47
3:N:332:ASN:HD21	3:N:355:ALA:HA	1.78	0.47
5:P:65:LEU:C	5:P:65:LEU:HD12	2.40	0.47
10:U:51:TYR:C	10:U:51:TYR:CD2	2.92	0.47
10:J:61:ASN:HD22	10:J:62:PRO:N	2.12	0.47
4:O:213:ASN:HB3	13:X:1:GLC:O4	2.14	0.47
3:C:184:TYR:CD1	16:C:4001:HEM:HBC1	2.49	0.47
11:V:50:TYR:O	11:V:51:THR:HG22	2.13	0.47
20:C:4033:CN5:H3FB	14:L:4113:6PH:H29A	1.96	0.47
10:J:61:ASN:ND2	10:J:63:SER:H	2.13	0.47
4:D:203:PRO:HG2	4:D:206:VAL:CG2	2.43	0.47
5:E:112:GLN:O	5:E:114:LYS:HD3	2.14	0.47
5:P:94:VAL:N	24:P:7409:HOH:O	2.46	0.47
2:B:40:ARG:HG3	2:B:155:LEU:HG	1.95	0.47
2:B:106:ALA:HA	2:B:206:LEU:HD13	1.96	0.47
3:C:147:ILE:HA	3:C:150:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:323:LYS:HE3	8:H:55:GLN:HE22	1.80	0.47
9:T:50:LYS:HG3	24:T:6999:HOH:O	2.13	0.47
10:U:36:ASN:OD1	10:U:51:TYR:HB3	2.15	0.47
11:V:34:ASN:ND2	11:V:49:TYR:HA	2.29	0.47
11:K:21:ILE:HG22	11:K:22:SER:N	2.30	0.47
11:K:90:HIS:HD2	11:K:92:ILE:HG22	1.80	0.47
2:M:230:ARG:HE	2:M:359:VAL:HG13	1.80	0.47
6:Q:92:LYS:HA	6:Q:95:VAL:HG22	1.96	0.47
2:B:324:LYS:O	2:B:327:VAL:HG22	2.14	0.47
4:D:268:ARG:NH1	9:I:33:ASP:OD1	2.48	0.47
11:K:34:ASN:HD21	11:K:91:HIS:HE1	1.63	0.47
1:L:164:LEU:HD13	1:L:327:LEU:HD13	1.97	0.47
1:L:172:THR:HG23	1:L:173:PRO:HD2	1.97	0.47
2:B:139:VAL:HG22	24:B:8522:HOH:O	2.15	0.47
4:D:69:LEU:HD11	6:F:131:GLN:HB3	1.96	0.47
5:E:132:VAL:HG21	5:E:192:ARG:NH1	2.30	0.47
5:P:43:LEU:HD21	8:S:29:VAL:HG11	1.97	0.47
11:V:19:VAL:HG12	11:V:78:LEU:HD11	1.97	0.47
2:B:152:ARG:HD3	2:B:224:PHE:CE1	2.50	0.46
3:C:143:GLY:O	3:C:147:ILE:HG12	2.15	0.46
9:I:3:PHE:CE1	9:I:5:SER:HB2	2.50	0.46
10:J:48:TRP:CZ2	10:J:50:GLY:HA2	2.50	0.46
2:B:49:HIS:HA	2:B:82:LEU:HD22	1.98	0.46
2:B:205:LEU:HD23	24:B:7883:HOH:O	2.16	0.46
5:P:65:LEU:CD1	9:T:25:ALA:HA	2.45	0.46
3:C:77:ILE:O	3:C:81:LEU:HB2	2.15	0.46
4:D:296:LYS:HE3	24:D:5128:HOH:O	2.15	0.46
5:E:43:LEU:HD21	8:H:29:VAL:HG11	1.97	0.46
2:M:89:LEU:N	2:M:89:LEU:HD12	2.31	0.46
2:M:228:GLU:HA	2:M:353:TYR:O	2.15	0.46
4:O:134:TYR:OH	4:O:156:PRO:HD3	2.16	0.46
11:V:93:LYS:NZ	11:V:93:LYS:HB3	2.30	0.46
1:A:283:GLN:NE2	1:A:373:GLN:NE2	2.63	0.46
4:D:113:ARG:NH1	24:D:5360:HOH:O	2.48	0.46
2:M:315:SER:O	2:M:318:ILE:HG22	2.15	0.46
1:A:156:HIS:HD2	1:A:159:ARG:NH2	2.13	0.46
3:C:57:ASN:HA	3:C:173:ASN:HD21	1.80	0.46
3:C:142:TRP:CH2	5:P:165:VAL:HG23	2.51	0.46
5:E:45:GLU:HB3	5:E:47:ASN:ND2	2.31	0.46
22:N:4131:CN3:HAA	7:R:85:HIS:CE1	2.51	0.46
21:O:4114:7PH:H2AA	21:O:4114:7PH:H25	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:48:SER:C	8:S:50:ARG:H	2.23	0.46
10:U:61:ASN:HD22	10:U:62:PRO:N	2.13	0.46
20:C:4033:CN5:H2A	3:N:199:MET:HG2	1.97	0.46
8:S:35:LYS:O	8:S:37:LEU:N	2.49	0.45
2:B:44:LYS:HB2	2:B:47:VAL:CG2	2.47	0.45
5:E:55:TYR:O	5:E:59:MET:HG2	2.16	0.45
1:L:283:GLN:NE2	1:L:373:GLN:NE2	2.63	0.45
2:M:84:ARG:HD2	2:M:159:LEU:HD13	1.99	0.45
1:A:66:ASN:HD22	1:A:66:ASN:H	1.65	0.45
2:B:35:VAL:HG12	2:B:179:VAL:HG12	1.99	0.45
1:L:130:ASN:HD22	1:L:130:ASN:N	2.14	0.45
1:L:207:VAL:HG11	1:L:394:VAL:CG2	2.45	0.45
3:N:203:ILE:HB	8:S:8:THR:HG21	1.98	0.45
4:O:286:TRP:CZ3	5:P:56:ALA:HA	2.51	0.45
2:B:68:VAL:O	2:B:72:GLU:HG3	2.17	0.45
2:B:152:ARG:HD2	24:B:8523:HOH:O	2.17	0.45
1:L:289:ASN:ND2	1:L:291:PHE:H	2.14	0.45
2:B:69:ARG:NH1	7:R:121:ASP:OD1	2.49	0.45
4:D:286:TRP:CD2	5:E:59:MET:HG3	2.52	0.45
3:N:117:GLY:O	16:N:4022:HEM:HMC3	2.16	0.45
1:A:80:LYS:HE2	2:B:263:ALA:HA	1.97	0.45
1:L:47:HIS:CE1	2:M:22:ARG:HH22	2.35	0.45
1:L:67:ASN:ND2	1:L:181:THR:HG23	2.31	0.45
2:M:146:LEU:HD13	2:M:354:VAL:HG22	1.99	0.45
10:U:21:THR:HG22	10:U:80:PHE:CD2	2.49	0.45
2:B:193:VAL:HG22	24:B:7468:HOH:O	2.15	0.45
2:M:71:SER:HA	2:M:74:LEU:HD12	1.99	0.45
10:U:37:TRP:CZ3	10:U:96:CYS:HB3	2.52	0.45
3:C:48:ILE:HD13	3:N:185:LEU:HG	1.98	0.44
3:C:95:MET:HG2	18:C:4010:8PE:H37A	1.99	0.44
11:K:14:SER:HB2	11:K:17:ASP:OD2	2.17	0.44
2:M:74:LEU:HD13	2:M:101:TYR:OH	2.18	0.44
3:N:18:ILE:HA	3:N:222:HIS:HB2	1.99	0.44
8:H:3:PRO:HG3	8:S:12:TRP:CE2	2.52	0.44
2:M:52:ASN:HD22	2:M:87:ILE:HG23	1.82	0.44
5:P:168:GLY:HA2	5:P:176:TRP:CD1	2.52	0.44
1:L:37:VAL:HG13	1:L:207:VAL:HA	2.00	0.44
2:M:44:LYS:HB2	2:M:47:VAL:CG2	2.47	0.44
3:N:216:LEU:N	3:N:216:LEU:HD12	2.33	0.44
15:A:4021:UMQ:O1'	9:I:18:VAL:HG13	2.17	0.44
7:G:18:SER:OG	7:G:21:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:57:SER:O	1:L:102:GLN:HB2	2.18	0.44
1:L:184:SER:O	1:L:188:LEU:HD13	2.17	0.44
1:A:39:ALA:HB1	1:A:390:LEU:HD11	1.99	0.44
1:A:60:ALA:O	1:A:173:PRO:HB3	2.17	0.44
2:B:318:ILE:HD13	2:B:343:VAL:HG22	1.99	0.44
5:E:208:ASP:O	5:E:211:LYS:HG2	2.17	0.44
7:R:80:GLN:O	7:R:84:THR:HG23	2.17	0.44
1:A:121:ASN:HD22	1:A:125:ILE:HD12	1.81	0.44
3:C:52:MET:HE3	3:N:178:ARG:CB	2.46	0.44
1:L:58:GLY:H	1:L:61:ASN:ND2	2.14	0.44
1:L:73:TRP:HA	1:L:76:ILE:HD11	1.99	0.44
2:B:66:LYS:O	2:B:70:GLU:HB2	2.18	0.44
10:J:21:THR:HG22	10:J:80:PHE:CD2	2.52	0.44
10:J:87:THR:HG22	10:J:88:THR:N	2.32	0.44
11:K:34:ASN:ND2	11:K:50:TYR:H	2.16	0.44
1:A:72:LEU:HD13	1:A:144:VAL:HG21	2.00	0.44
1:A:270:VAL:HG21	1:A:396:ILE:HD13	2.00	0.44
3:C:52:MET:HE1	5:E:82:MET:CG	2.35	0.44
10:J:107:TYR:H	11:K:91:HIS:CD2	2.36	0.44
4:O:136:ASP:HB3	4:O:145:LYS:HG3	2.00	0.44
12:W:46:GLY:HA2	12:W:53:TYR:CE1	2.53	0.44
5:E:45:GLU:HG2	5:E:46:ASN:H	1.81	0.44
11:K:15:LEU:HD12	11:K:15:LEU:N	2.33	0.44
11:K:90:HIS:CD2	11:K:92:ILE:HG22	2.52	0.44
3:N:173:ASN:HB3	3:N:174:PRO:HD3	2.00	0.44
1:A:69:VAL:HG23	1:A:193:LEU:HD22	2.00	0.43
1:A:169:PHE:O	1:A:175:SER:HB3	2.18	0.43
1:A:380:SER:HB3	24:A:7013:HOH:O	2.17	0.43
10:J:40:LEU:HB3	10:J:93:THR:OG1	2.18	0.43
10:J:59:ASN:C	10:J:59:ASN:HD22	2.26	0.43
1:L:349:LYS:HA	1:L:349:LYS:HE2	2.00	0.43
4:O:286:TRP:CD2	5:P:59:MET:HG3	2.53	0.43
1:A:152:GLU:HG3	24:A:6944:HOH:O	2.18	0.43
1:A:172:THR:CG2	1:A:242:ALA:HA	2.48	0.43
11:K:34:ASN:ND2	11:K:49:TYR:HA	2.33	0.43
3:N:76:TYR:CG	4:O:262:GLU:HG3	2.53	0.43
5:E:106:ASN:ND2	5:E:119:ARG:HB2	2.33	0.43
8:H:35:LYS:O	8:H:37:LEU:N	2.46	0.43
11:V:6:GLN:HG2	11:V:23:CYS:SG	2.58	0.43
11:V:18:ARG:HD2	11:V:18:ARG:C	2.43	0.43
2:B:62:ARG:HH21	2:B:62:ARG:CG	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:SER:HB2	2:B:316:PRO:HD3	2.00	0.43
4:D:277:LEU:HD21	21:D:4014:7PH:H34	2.00	0.43
5:E:72:LYS:NZ	9:I:29:GLN:HE22	2.16	0.43
10:J:13:GLN:HA	10:J:121:SER:O	2.18	0.43
1:L:72:LEU:HD12	1:L:72:LEU:HA	1.88	0.43
1:L:430:ASP:OD2	1:L:449:ARG:NH2	2.48	0.43
2:M:124:LEU:HB3	2:M:128:ARG:NH2	2.33	0.43
7:G:120:LEU:HA	7:G:123:ILE:HG23	2.01	0.43
1:A:169:PHE:O	1:A:172:THR:HB	2.19	0.43
5:P:187:ILE:O	5:P:187:ILE:HG13	2.19	0.43
8:S:48:SER:O	8:S:49:PHE:HB2	2.18	0.43
11:V:27:GLN:HG2	11:V:28:ASP:N	2.34	0.43
12:W:65:ASP:H	12:W:68:ASN:ND2	2.14	0.43
1:A:38:VAL:HA	1:A:208:VAL:HG13	2.01	0.43
22:D:4031:CN3:HC	24:D:6590:HOH:O	2.19	0.43
1:L:227:ASN:N	1:L:227:ASN:HD22	2.17	0.43
1:L:252:ARG:HD2	8:S:21:GLN:HB2	2.00	0.43
12:W:10:LYS:HB2	12:W:10:LYS:NZ	2.33	0.43
3:C:362:TYR:O	3:C:367:VAL:HG23	2.19	0.43
11:K:92:ILE:HD13	11:K:92:ILE:O	2.18	0.43
2:M:318:ILE:HG23	2:M:319:ASN:N	2.34	0.43
3:C:312:VAL:HG21	7:G:5:PHE:CZ	2.53	0.43
10:J:49:VAL:HG12	10:J:68:LEU:HD23	2.01	0.43
11:K:63:SER:HB2	11:K:74:THR:HB	2.01	0.43
1:L:62:GLU:OE1	1:L:67:ASN:HA	2.18	0.43
3:N:58:ILE:HB	3:N:173:ASN:HA	2.01	0.43
8:S:47:ASN:O	8:S:50:ARG:HB3	2.19	0.43
10:U:109:MET:HE3	11:V:96:TRP:CZ3	2.54	0.43
2:B:146:LEU:HD12	2:B:146:LEU:HA	1.87	0.42
2:M:251:ALA:CB	2:M:339:ASN:HB2	2.49	0.42
4:O:225:MET:CE	24:O:5654:HOH:O	2.59	0.42
10:U:38:ILE:CD1	10:U:46:LEU:HD22	2.49	0.42
2:B:152:ARG:HG2	2:M:364:TYR:CZ	2.55	0.42
3:C:216:LEU:HD12	3:C:216:LEU:N	2.34	0.42
5:E:103:LEU:O	5:E:120:HIS:O	2.37	0.42
8:H:41:PHE:O	8:H:42:HIS:HB3	2.19	0.42
2:M:317:ALA:O	2:M:321:THR:HG22	2.18	0.42
11:V:31:ASN:HD22	11:V:51:THR:HG21	1.84	0.42
3:C:25:SER:OG	7:G:79:HIS:HD2	2.02	0.42
3:C:173:ASN:HB3	3:C:174:PRO:HD3	2.01	0.42
1:L:127:GLN:HB3	1:L:130:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:203:PRO:O	5:P:205:TYR:HD1	2.02	0.42
11:V:2:ILE:HD12	11:V:2:ILE:N	2.29	0.42
2:B:35:VAL:HG12	2:B:179:VAL:CG1	2.50	0.42
1:L:315:PHE:CD1	1:L:315:PHE:C	2.97	0.42
8:S:41:PHE:C	8:S:43:ASN:H	2.26	0.42
12:W:68:ASN:HD22	12:W:68:ASN:C	2.27	0.42
1:L:349:LYS:HE2	1:L:352:ASN:OD1	2.20	0.42
2:M:40:ARG:HA	2:M:154:GLY:O	2.19	0.42
3:N:25:SER:OG	7:R:79:HIS:HD2	2.03	0.42
4:D:301:VAL:CG2	8:H:25:THR:HB	2.50	0.42
1:L:235:LYS:NZ	1:L:235:LYS:HB2	2.35	0.42
3:N:157:VAL:O	3:N:161:ILE:HG12	2.20	0.42
2:M:59:THR:HA	2:M:112:THR:HA	2.02	0.42
3:N:77:ILE:O	3:N:81:LEU:HB2	2.19	0.42
10:U:34:TYR:HB2	10:U:99:SER:OG	2.20	0.42
10:J:24:VAL:CG2	10:J:29:ILE:HD11	2.49	0.42
1:L:209:VAL:HG13	1:L:390:LEU:HD13	2.02	0.42
2:M:326:ALA:C	2:M:328:GLN:H	2.27	0.42
22:N:4131:CN3:CC	24:O:6998:HOH:O	2.68	0.42
7:R:45:PHE:O	7:R:48:LEU:HB2	2.19	0.42
10:U:48:TRP:CZ2	10:U:50:GLY:HA2	2.54	0.42
10:U:98:ARG:O	10:U:109:MET:HA	2.19	0.42
2:B:141:SER:HB2	24:B:7070:HOH:O	2.19	0.42
3:N:165:LEU:O	3:N:178:ARG:HD2	2.20	0.42
3:N:301:VAL:O	3:N:304:VAL:HG22	2.20	0.42
1:A:74:LYS:HG3	1:A:95:SER:HB3	2.01	0.41
2:B:362:LEU:HD12	2:B:362:LEU:HA	1.90	0.41
11:K:4:LEU:N	11:K:4:LEU:HD12	2.34	0.41
5:P:85:THR:O	5:P:88:VAL:HG22	2.20	0.41
1:A:57:SER:O	1:A:102:GLN:HB2	2.20	0.41
1:A:145:LEU:HD11	1:A:185:LEU:HB3	2.01	0.41
1:A:169:PHE:HB3	1:A:172:THR:HG22	2.02	0.41
2:B:230:ARG:NE	2:B:359:VAL:HG13	2.34	0.41
2:B:255:VAL:HG23	2:B:314:LEU:HD13	2.02	0.41
10:J:51:TYR:C	10:J:51:TYR:HD2	2.28	0.41
2:M:98:LEU:N	2:M:99:PRO:HD2	2.35	0.41
5:P:58:PHE:CD2	5:P:59:MET:HE2	2.54	0.41
4:O:296:LYS:HE3	24:O:5628:HOH:O	2.19	0.41
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.85	0.41
3:N:295:MET:SD	17:N:4025:SMA:H1	2.60	0.41
14:A:4013:6PH:H38	3:C:230:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:PHE:CZ	3:C:125:ILE:HD11	2.55	0.41
11:K:34:ASN:ND2	11:K:91:HIS:HE1	2.18	0.41
2:M:112:THR:OG1	2:M:114:PHE:CE2	2.74	0.41
3:N:20:SER:HA	3:N:21:PRO:HD3	1.93	0.41
10:U:18:LEU:O	10:U:82:LYS:HA	2.20	0.41
11:V:15:LEU:HD12	11:V:15:LEU:N	2.34	0.41
11:V:32:PHE:HB2	11:V:92:ILE:HG22	2.03	0.41
3:C:117:GLY:O	16:C:4002:HEM:HMC3	2.21	0.41
3:C:214:GLY:O	3:C:218:ARG:CD	2.69	0.41
1:L:115:LYS:HA	1:L:115:LYS:HD2	1.88	0.41
2:M:254:GLU:HG2	2:M:276:LEU:HD23	2.02	0.41
3:N:48:ILE:HD12	3:N:184:TYR:OH	2.21	0.41
3:N:93:MET:HE2	16:N:4022:HEM:HAB	2.02	0.41
7:R:18:SER:OG	7:R:21:LEU:HD23	2.20	0.41
11:V:21:ILE:HG22	11:V:22:SER:N	2.35	0.41
11:V:53:ARG:HG3	11:V:53:ARG:NH2	2.35	0.41
1:A:172:THR:HG23	1:A:242:ALA:HA	2.03	0.41
2:B:315:SER:HG	2:B:344:LYS:HD2	1.84	0.41
10:J:76:LYS:HB2	10:J:78:GLN:HG2	2.02	0.41
1:L:241:LYS:HD2	1:L:241:LYS:N	2.35	0.41
2:M:230:ARG:NE	2:M:359:VAL:HG13	2.35	0.41
2:M:312:LYS:HE2	2:M:312:LYS:HB3	1.75	0.41
3:N:166:TRP:CE3	3:N:170:SER:HA	2.54	0.41
1:A:364:GLU:HG3	7:R:125:VAL:HG21	2.03	0.41
2:B:193:VAL:HG23	2:B:193:VAL:O	2.21	0.41
2:B:230:ARG:HE	2:B:359:VAL:HG13	1.85	0.41
3:C:147:ILE:HD12	17:C:4005:SMA:H14	2.02	0.41
5:E:165:VAL:HG23	3:N:142:TRP:CH2	2.56	0.41
11:K:48:ILE:HD13	11:K:54:LEU:HA	2.03	0.41
1:L:74:LYS:HG3	1:L:95:SER:HB3	2.01	0.41
1:L:289:ASN:HD22	1:L:291:PHE:H	1.69	0.41
1:L:424:LYS:HD2	1:L:424:LYS:HA	1.94	0.41
2:M:337:GLU:C	2:M:339:ASN:H	2.26	0.41
4:O:111:ALA:HA	4:O:154:TYR:HA	2.02	0.41
8:S:49:PHE:O	8:S:53:LYS:HB2	2.21	0.41
8:H:2:GLY:HA2	8:H:3:PRO:HD3	1.83	0.41
10:J:67:ARG:HH12	10:J:90:ASP:CG	2.28	0.41
7:R:91:ASN:HD22	7:R:91:ASN:H	1.69	0.41
10:U:109:MET:HE3	11:V:96:TRP:HZ3	1.86	0.41
11:V:2:ILE:H	11:V:2:ILE:CD1	2.32	0.41
2:B:336:ILE:HD12	2:B:336:ILE:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:139:MET:HA	3:C:139:MET:HE2	2.02	0.40
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.60	0.40
2:M:197:LEU:O	2:M:201:VAL:HG23	2.20	0.40
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.35	0.40
1:A:179:ARG:NH2	1:A:179:ARG:CG	2.81	0.40
1:A:228:LEU:HG	1:A:229:SER:N	2.36	0.40
2:M:50:LEU:HD23	2:M:50:LEU:HA	1.92	0.40
16:N:4021:HEM:HHD	16:N:4021:HEM:HBC2	2.02	0.40
2:B:112:THR:OG1	2:B:114:PHE:CE2	2.74	0.40
2:B:146:LEU:HG	2:B:242:GLY:HA3	2.03	0.40
2:B:164:VAL:CG2	2:M:232:ARG:NH1	2.84	0.40
3:C:104:GLY:HA2	3:C:106:TYR:CE2	2.56	0.40
2:B:181:THR:HB	2:B:212:GLY:H	1.86	0.40
3:C:32:MET:HE2	3:C:95:MET:HB2	2.03	0.40
5:E:106:ASN:HD21	5:E:119:ARG:HD2	1.86	0.40
1:L:43:ASN:HA	1:L:44:PRO:HD2	1.92	0.40
1:L:228:LEU:O	1:L:228:LEU:HD12	2.22	0.40
2:M:137:CYS:HA	2:M:138:PRO:HD2	1.93	0.40
7:R:100:VAL:HG13	7:R:101:PRO:HD2	2.02	0.40
8:S:7:LYS:HA	8:S:7:LYS:HD3	1.84	0.40
11:V:33:LEU:HD13	11:V:71:TYR:CD1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	408 (95%)	19 (4%)	2 (0%)	24	16
1	L	429/431 (100%)	406 (95%)	19 (4%)	4 (1%)	14	6
2	B	350/352 (99%)	330 (94%)	15 (4%)	5 (1%)	9	3
2	M	350/352 (99%)	330 (94%)	19 (5%)	1 (0%)	36	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	383/385 (100%)	370 (97%)	12 (3%)	1 (0%)	36	29
3	N	383/385 (100%)	369 (96%)	13 (3%)	1 (0%)	36	29
4	D	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
4	O	246/248 (99%)	241 (98%)	4 (2%)	1 (0%)	30	22
5	E	183/185 (99%)	173 (94%)	8 (4%)	2 (1%)	11	4
5	P	183/185 (99%)	169 (92%)	10 (6%)	4 (2%)	5	1
6	F	72/146 (49%)	71 (99%)	1 (1%)	0	100	100
6	Q	72/146 (49%)	70 (97%)	2 (3%)	0	100	100
7	G	124/126 (98%)	122 (98%)	2 (2%)	0	100	100
7	R	124/126 (98%)	123 (99%)	1 (1%)	0	100	100
8	H	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	11	4
8	S	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	11	4
9	I	55/65 (85%)	53 (96%)	2 (4%)	0	100	100
9	T	55/65 (85%)	52 (94%)	2 (4%)	1 (2%)	6	1
10	J	125/127 (98%)	114 (91%)	11 (9%)	0	100	100
10	U	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
11	K	105/107 (98%)	91 (87%)	10 (10%)	4 (4%)	2	0
11	V	105/107 (98%)	91 (87%)	11 (10%)	3 (3%)	3	0
12	W	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
All	All	4432/4638 (96%)	4206 (95%)	195 (4%)	31 (1%)	18	10

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	103	LEU
5	P	103	LEU
2	B	153	LYS
3	C	223	SER
1	L	228	LEU
3	N	223	SER
11	V	30	ASN
1	A	128	LYS
2	B	335	PRO
11	K	51	THR
1	L	232	THR

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	347 (94%)	23 (6%)	16	9
1	L	370/370 (100%)	341 (92%)	29 (8%)	11	5
2	B	301/301 (100%)	288 (96%)	13 (4%)	26	18
2	M	301/301 (100%)	282 (94%)	19 (6%)	16	8
3	C	338/338 (100%)	321 (95%)	17 (5%)	22	14
3	N	338/338 (100%)	322 (95%)	16 (5%)	23	15
4	D	206/206 (100%)	202 (98%)	4 (2%)	50	47
4	O	206/206 (100%)	203 (98%)	3 (2%)	57	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	151/151 (100%)	148 (98%)	3 (2%)	48	46
5	P	151/151 (100%)	144 (95%)	7 (5%)	24	16
6	F	67/130 (52%)	61 (91%)	6 (9%)	9	3
6	Q	67/130 (52%)	64 (96%)	3 (4%)	24	17
7	G	110/110 (100%)	103 (94%)	7 (6%)	16	8
7	R	110/110 (100%)	106 (96%)	4 (4%)	31	23
8	H	77/77 (100%)	75 (97%)	2 (3%)	40	35
8	S	77/77 (100%)	76 (99%)	1 (1%)	61	61
9	I	47/53 (89%)	47 (100%)	0	100	100
9	T	47/53 (89%)	45 (96%)	2 (4%)	26	18
10	J	112/112 (100%)	104 (93%)	8 (7%)	13	7
10	U	112/112 (100%)	106 (95%)	6 (5%)	20	12
11	K	93/93 (100%)	89 (96%)	4 (4%)	26	18
11	V	93/93 (100%)	89 (96%)	4 (4%)	26	18
12	W	89/88 (101%)	87 (98%)	2 (2%)	45	42
All	All	3833/3970 (96%)	3650 (95%)	183 (5%)	23	15

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	120	LEU
1	A	145	LEU
1	A	164	LEU
1	A	172	THR
1	A	174	LEU
1	A	179	ARG
1	A	185	LEU
1	A	188	LEU
1	A	193	LEU
1	A	239	LYS
1	A	240	LYS
1	A	241	LYS
1	A	311	LEU
1	A	320	LEU
1	A	330	PHE
1	A	343	LEU

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Mol	Chain	Res	Type
1	A	360	ASP
1	A	370	LEU
1	A	374	LEU
1	A	425	ARG
1	A	426	LEU
1	A	443	LEU
2	B	53	ARG
2	B	54	PHE
2	B	73	LEU
2	B	87	ILE
2	B	144	ASP
2	B	146	LEU
2	B	169	LEU
2	B	238	VAL
2	B	245	VAL
2	B	254	GLU
2	B	345	ASP
2	B	347	LYS
2	B	362	LEU
3	C	10	LEU
3	C	35	LEU
3	C	38	LEU
3	C	60	LEU
3	C	79	ARG
3	C	81	LEU
3	C	99	LYS
3	C	150	LEU
3	C	182	LEU
3	C	185	LEU
3	C	238	LEU
3	C	302	LEU
3	C	313	VAL
3	C	336	LEU
3	C	347	PRO
3	C	350	LEU
3	C	377	LEU
4	D	69	LEU
4	D	251	VAL
4	D	280	LEU
4	D	283	LEU
5	E	65	LEU
5	E	110	LYS

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Mol	Chain	Res	Type
5	E	114	LYS
6	F	77	GLN
6	F	89	GLU
6	F	94	LEU
6	F	99	GLU
6	F	130	LEU
6	F	131	GLN
7	G	2	PRO
7	G	16	LEU
7	G	31	GLN
7	G	62	ARG
7	G	91	ASN
7	G	97	GLN
7	G	127	LYS
8	H	60	LEU
8	H	89	LEU
10	J	36	ASN
10	J	38	ILE
10	J	39	ARG
10	J	51	TYR
10	J	59	ASN
10	J	61	ASN
10	J	68	LEU
10	J	114	GLN
11	K	38	GLN
11	K	81	GLU
11	K	92	ILE
11	K	93	LYS
1	L	66	ASN
1	L	72	LEU
1	L	76	ILE
1	L	120	LEU
1	L	130	ASN
1	L	145	LEU
1	L	150	ASP
1	L	152	GLU
1	L	164	LEU
1	L	172	THR
1	L	174	LEU
1	L	176	LEU
1	L	185	LEU
1	L	188	LEU

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Mol	Chain	Res	Type
1	L	213	ASN
1	L	214	ILE
1	L	228	LEU
1	L	241	LYS
1	L	261	ILE
1	L	311	LEU
1	L	320	LEU
1	L	330	PHE
1	L	343	LEU
1	L	370	LEU
1	L	374	LEU
1	L	390	LEU
1	L	425	ARG
1	L	426	LEU
1	L	443	LEU
2	M	17	LEU
2	M	53	ARG
2	M	54	PHE
2	M	73	LEU
2	M	74	LEU
2	M	144	ASP
2	M	146	LEU
2	M	169	LEU
2	M	206	LEU
2	M	218	LYS
2	M	238	VAL
2	M	246	ASN
2	M	250	LEU
2	M	254	GLU
2	M	270	LEU
2	M	292	GLN
2	M	312	LYS
2	M	330	GLU
2	M	362	LEU
3	N	35	LEU
3	N	38	LEU
3	N	99	LYS
3	N	101	LEU
3	N	109	PRO
3	N	150	LEU
3	N	182	LEU
3	N	185	LEU

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Mol	Chain	Res	Type
3	N	238	LEU
3	N	283	ARG
3	N	312	VAL
3	N	313	VAL
3	N	335	LEU
3	N	336	LEU
3	N	350	LEU
3	N	377	LEU
4	O	69	LEU
4	O	280	LEU
4	O	283	LEU
5	P	41	ASP
5	P	44	LYS
5	P	45	GLU
5	P	65	LEU
5	P	107	VAL
5	P	110	LYS
5	P	211	LYS
6	Q	77	GLN
6	Q	94	LEU
6	Q	103	GLU
7	R	2	PRO
7	R	16	LEU
7	R	41	LEU
7	R	62	ARG
8	S	87	GLU
9	T	18	VAL
9	T	48	LEU
10	U	38	ILE
10	U	39	ARG
10	U	61	ASN
10	U	68	LEU
10	U	114	GLN
10	U	118	VAL
11	V	18	ARG
11	V	81	GLU
11	V	92	ILE
11	V	93	LYS
12	W	10	LYS
12	W	68	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) 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	121	ASN
1	A	126	GLN
1	A	156	HIS
1	A	170	GLN
1	A	213	ASN
1	A	283	GLN
1	A	289	ASN
1	A	305	ASN
1	A	314	ASN
1	A	317	HIS
1	A	336	ASN
1	A	350	GLN
1	A	373	GLN
1	A	385	ASN
1	A	429	GLN
2	B	49	HIS
2	B	52	ASN
2	B	55	ASN
2	B	57	GLN
2	B	191	ASN
2	B	258	ASN
2	B	339	ASN
3	C	14	ASN
3	C	74	ASN
3	C	173	ASN
3	C	177	GLN
3	C	204	HIS
3	C	208	ASN
3	C	253	HIS
3	C	332	ASN
3	C	343	HIS
4	D	78	HIS
4	D	79	ASN
4	D	127	ASN
4	D	143	ASN
5	E	38	ASN
5	E	47	ASN
5	E	106	ASN

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Mol	Chain	Res	Type
5	E	127	GLN
5	E	184	HIS
6	F	77	GLN
6	F	109	GLN
6	F	110	GLN
6	F	129	HIS
6	F	131	GLN
7	G	31	GLN
7	G	53	ASN
7	G	79	HIS
7	G	91	ASN
7	G	97	GLN
8	H	43	ASN
8	H	47	ASN
9	I	14	ASN
9	I	29	GLN
10	J	54	ASN
10	J	59	ASN
10	J	61	ASN
10	J	77	ASN
10	J	78	GLN
10	J	114	GLN
11	K	27	GLN
11	K	30	ASN
11	K	31	ASN
11	K	34	ASN
11	K	38	GLN
11	K	77	ASN
11	K	89	GLN
11	K	90	HIS
11	K	91	HIS
1	L	31	GLN
1	L	47	HIS
1	L	61	ASN
1	L	66	ASN
1	L	67	ASN
1	L	102	GLN
1	L	122	GLN
1	L	127	GLN
1	L	130	ASN
1	L	156	HIS
1	L	170	GLN

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Mol	Chain	Res	Type
1	L	213	ASN
1	L	227	ASN
1	L	271	ASN
1	L	283	GLN
1	L	289	ASN
1	L	317	HIS
1	L	336	ASN
1	L	385	ASN
2	M	49	HIS
2	M	52	ASN
2	M	55	ASN
2	M	57	GLN
2	M	170	GLN
2	M	246	ASN
2	M	252	GLN
2	M	292	GLN
3	N	14	ASN
3	N	43	GLN
3	N	74	ASN
3	N	173	ASN
3	N	177	GLN
3	N	208	ASN
3	N	253	HIS
3	N	332	ASN
4	O	78	HIS
4	O	79	ASN
4	O	127	ASN
4	O	170	GLN
5	P	46	ASN
5	P	97	ASN
5	P	106	ASN
5	P	124	HIS
5	P	127	GLN
5	P	184	HIS
6	Q	77	GLN
6	Q	109	GLN
6	Q	119	HIS
7	R	30	ASN
7	R	53	ASN
7	R	79	HIS
7	R	91	ASN
8	S	38	GLN

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Mol	Chain	Res	Type
8	S	55	GLN
9	T	14	ASN
9	T	29	GLN
10	U	54	ASN
10	U	61	ASN
10	U	77	ASN
10	U	78	GLN
10	U	114	GLN
11	V	30	ASN
11	V	31	ASN
11	V	34	ASN
11	V	38	GLN
11	V	55	HIS
11	V	77	ASN
11	V	89	GLN
11	V	91	HIS
12	W	44	HIS
12	W	67	ASN
12	W	68	ASN
12	W	75	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	M3L	W	77	12	10,11,12	0.92	0	9,14,16	0.99	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	M3L	W	77	12	-	0/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	W	77	M3L	CM2-NZ-CM1	-2.03	103.64	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	0.62	0	15,15,17	0.79	1 (6%)
13	FRU	X	2	13	11,12,12	0.52	0	10,18,18	0.54	0

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

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
13	X	1	GLC	C2-C3-C4	-2.81	105.92	110.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

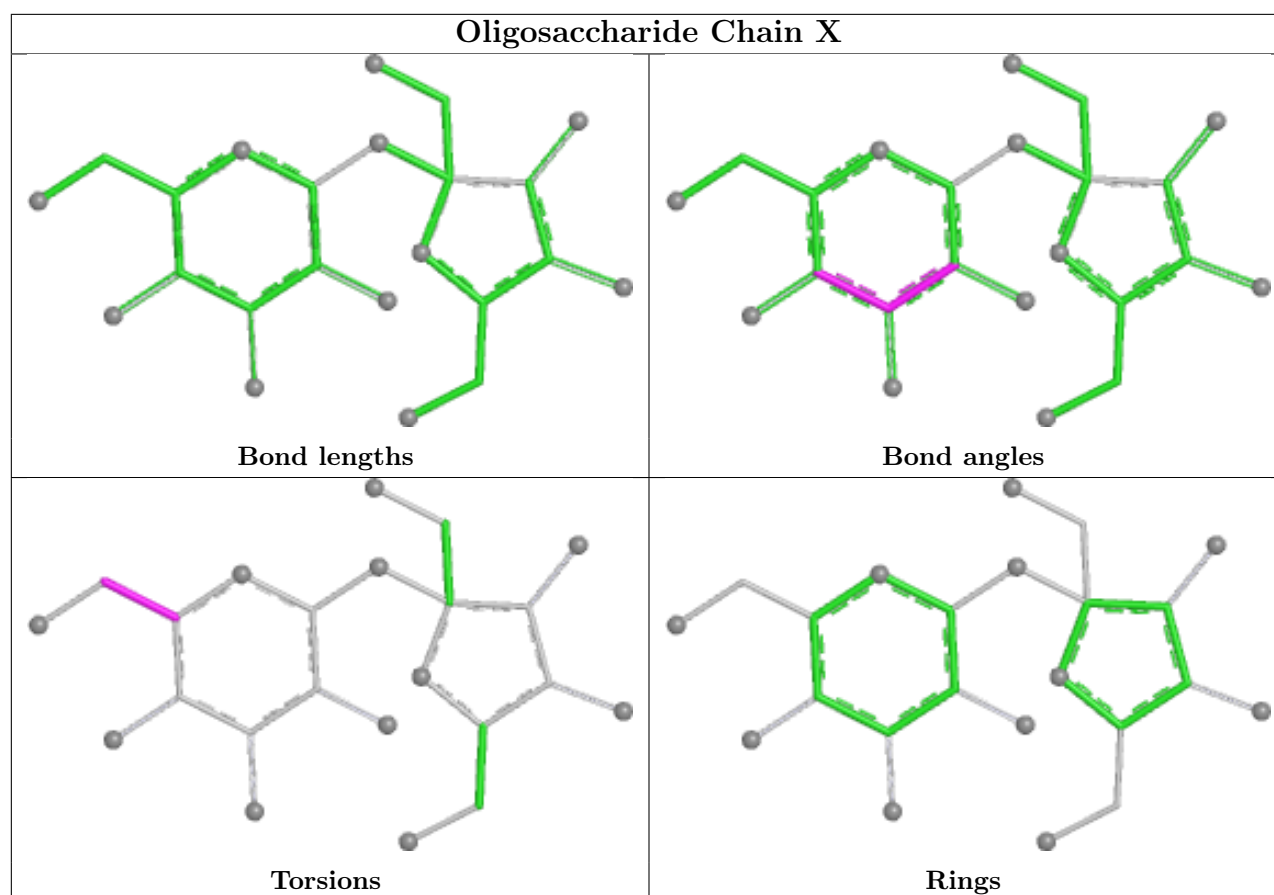
Mol	Chain	Res	Type	Atoms
13	X	1	GLC	C4-C5-C6-O6
13	X	1	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

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



5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	9PE	C	4011	-	39,39,39	0.71	0	42,44,44	0.97	1 (2%)
22	CN3	D	4031	-	54,54,54	1.54	9 (16%)	60,66,66	1.52	9 (15%)
21	7PH	D	4014	-	37,37,37	1.01	1 (2%)	40,42,42	1.44	8 (20%)
18	8PE	C	4010	-	46,46,46	0.96	2 (4%)	49,51,51	1.19	2 (4%)
14	6PH	L	4113	-	39,39,39	0.99	2 (5%)	42,44,44	1.34	4 (9%)
23	FES	P	4024	5	0,4,4	-	-	-	-	-
14	6PH	A	4013	-	39,39,39	0.99	3 (7%)	42,44,44	1.31	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	9PE	N	4111	-	39,39,39	0.75	0	42,44,44	1.00	1 (2%)
16	HEM	D	4003	4	50,50,50	1.42	5 (10%)	67,82,82	0.84	3 (4%)
16	HEM	C	4001	3	50,50,50	1.36	9 (18%)	67,82,82	0.91	4 (5%)
16	HEM	W	4026	12	50,50,50	1.48	7 (14%)	67,82,82	0.96	5 (7%)
16	HEM	N	4021	3	50,50,50	1.41	11 (22%)	67,82,82	0.92	3 (4%)
22	CN3	N	4131	-	54,54,54	1.52	10 (18%)	60,66,66	1.50	9 (15%)
16	HEM	C	4002	3	50,50,50	1.31	7 (14%)	67,82,82	0.68	0
17	SMA	N	4025	-	38,38,38	0.78	1 (2%)	47,52,52	0.94	3 (6%)
15	UMQ	A	4021	-	35,35,35	0.92	1 (2%)	46,46,46	1.78	7 (15%)
16	HEM	N	4022	3	50,50,50	1.34	7 (14%)	67,82,82	0.76	0
16	HEM	O	4023	4	50,50,50	1.49	7 (14%)	67,82,82	0.83	2 (2%)
21	7PH	O	4114	-	37,37,37	1.01	1 (2%)	40,42,42	1.44	8 (20%)
20	CN5	C	4033	-	40,40,40	1.68	11 (27%)	44,48,48	1.84	9 (20%)
17	SMA	C	4005	-	38,38,38	0.78	0	47,52,52	0.94	4 (8%)
23	FES	E	4004	5	0,4,4	-	-	-	-	-
18	8PE	N	4110	-	46,46,46	0.99	3 (6%)	49,51,51	1.15	2 (4%)
15	UMQ	L	4121	-	35,35,35	0.95	1 (2%)	46,46,46	1.75	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	9PE	C	4011	-	-	21/43/43/43	-
22	CN3	D	4031	-	-	28/65/65/65	-
21	7PH	D	4014	-	-	13/39/39/39	-
18	8PE	C	4010	-	-	17/50/50/50	-
14	6PH	L	4113	-	-	19/41/41/41	-
23	FES	P	4024	5	-	-	0/1/1/1
14	6PH	A	4013	-	-	17/41/41/41	-
19	9PE	N	4111	-	-	17/43/43/43	-
16	HEM	D	4003	4	-	8/14/54/54	-
16	HEM	C	4001	3	-	4/14/54/54	-
16	HEM	W	4026	12	-	5/14/54/54	-
16	HEM	N	4021	3	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CN3	N	4131	-	-	29/65/65/65	-
16	HEM	C	4002	3	-	4/14/54/54	-
17	SMA	N	4025	-	-	1/34/34/34	0/2/2/2
15	UMQ	A	4021	-	-	4/20/60/60	0/2/2/2
16	HEM	N	4022	3	-	4/14/54/54	-
16	HEM	O	4023	4	-	8/14/54/54	-
21	7PH	O	4114	-	-	12/39/39/39	-
20	CN5	C	4033	-	-	18/44/44/44	-
17	SMA	C	4005	-	-	3/34/34/34	0/2/2/2
23	FES	E	4004	5	-	-	0/1/1/1
18	8PE	N	4110	-	-	21/50/50/50	-
15	UMQ	L	4121	-	-	4/20/60/60	0/2/2/2

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	4003	HEM	CBC-CAC	5.00	1.54	1.30
16	O	4023	HEM	CBC-CAC	5.00	1.54	1.30
16	O	4023	HEM	CBB-CAB	4.91	1.54	1.30
16	W	4026	HEM	CBC-CAC	4.83	1.53	1.30
16	D	4003	HEM	CBB-CAB	4.81	1.53	1.30
16	W	4026	HEM	CBB-CAB	4.68	1.52	1.30
22	D	4031	CN3	O31-C3	-4.41	1.35	1.45
22	N	4131	CN3	O31-C3	-4.39	1.35	1.45
20	C	4033	CN5	P-O14	3.81	1.64	1.50
22	D	4031	CN3	O21-C2	-3.73	1.37	1.46
16	C	4002	HEM	CBB-CAB	3.72	1.48	1.30
21	D	4014	7PH	O31-C3	-3.62	1.37	1.45
22	D	4031	CN3	O3'-CA	-3.58	1.31	1.44
22	N	4131	CN3	O21-C2	-3.57	1.38	1.46
21	O	4114	7PH	O31-C3	-3.51	1.37	1.45
22	N	4131	CN3	O3'-CA	-3.50	1.31	1.44
20	C	4033	CN5	O3'-CA	-3.44	1.31	1.44
18	C	4010	8PE	O21-C21	3.41	1.43	1.34
15	A	4021	UMQ	C3-C2	-3.38	1.43	1.52
15	L	4121	UMQ	C3-C2	-3.36	1.43	1.52
18	N	4110	8PE	O21-C21	3.32	1.43	1.34
16	N	4022	HEM	FE-NB	3.28	2.05	1.94
16	N	4022	HEM	CMC-C2C	3.19	1.57	1.50
16	N	4022	HEM	CBB-CAB	3.15	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	4033	CN5	P'-O2'	3.11	1.61	1.50
16	C	4001	HEM	CAC-C3C	-2.99	1.39	1.47
16	C	4002	HEM	CBC-CAC	2.97	1.44	1.30
16	N	4021	HEM	CAC-C3C	-2.97	1.39	1.47
16	C	4002	HEM	CMA-C3A	2.96	1.56	1.50
16	W	4026	HEM	FE-NA	2.93	2.04	1.95
16	C	4001	HEM	FE-NB	2.92	2.03	1.94
16	N	4021	HEM	FE-NB	2.91	2.03	1.94
20	C	4033	CN5	OA-CB	2.90	1.51	1.43
20	C	4033	CN5	P-O11	2.89	1.70	1.59
16	O	4023	HEM	FE-NC	2.82	2.04	1.95
16	N	4021	HEM	CBB-CAB	2.82	1.43	1.30
16	C	4001	HEM	FE-NC	2.80	2.04	1.95
16	C	4001	HEM	CBC-CAC	2.75	1.43	1.30
20	C	4033	CN5	CC-CB	2.75	1.60	1.51
22	N	4131	CN3	O32-C31	-2.75	1.14	1.22
16	N	4022	HEM	CBC-CAC	2.73	1.43	1.30
16	W	4026	HEM	FE-NB	2.72	2.03	1.94
16	N	4021	HEM	CBC-CAC	2.71	1.43	1.30
16	N	4021	HEM	CAB-C3B	-2.71	1.40	1.47
16	C	4001	HEM	CAB-C3B	-2.70	1.40	1.47
16	N	4021	HEM	FE-NC	2.67	2.04	1.95
16	O	4023	HEM	CAB-C3B	2.66	1.54	1.47
16	N	4021	HEM	FE-ND	2.66	2.03	1.94
22	D	4031	CN3	CC-CB	2.66	1.60	1.51
16	O	4023	HEM	FE-NB	2.65	2.03	1.94
22	D	4031	CN3	O11-C1	-2.64	1.34	1.44
16	N	4022	HEM	CMA-C3A	2.62	1.56	1.50
22	N	4131	CN3	CA-CB	2.61	1.59	1.51
16	W	4026	HEM	FE-ND	2.60	2.02	1.94
22	N	4131	CN3	CC-CB	2.58	1.59	1.51
22	N	4131	CN3	O21-C21	2.56	1.41	1.34
22	D	4031	CN3	O32-C31	-2.51	1.15	1.22
22	D	4031	CN3	O21-C21	2.51	1.41	1.34
22	D	4031	CN3	CA-CB	2.51	1.59	1.51
16	W	4026	HEM	FE-NC	2.51	2.03	1.95
16	D	4003	HEM	FE-NB	2.50	2.02	1.94
16	W	4026	HEM	CAB-C3B	2.48	1.54	1.47
16	C	4001	HEM	CMB-C2B	2.48	1.55	1.50
16	C	4001	HEM	CBB-CAB	2.47	1.42	1.30
22	N	4131	CN3	O11-C1	-2.47	1.35	1.44
16	C	4001	HEM	CMD-C2D	2.44	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	4021	HEM	CMD-C2D	2.43	1.55	1.50
16	D	4003	HEM	CAB-C3B	2.42	1.53	1.47
16	N	4021	HEM	CMB-C2B	2.40	1.55	1.50
16	O	4023	HEM	FE-NA	2.39	2.03	1.95
14	L	4113	6PH	C1-C2	2.39	1.58	1.50
16	O	4023	HEM	CAC-C3C	2.38	1.53	1.47
16	N	4022	HEM	CAB-C3B	-2.36	1.41	1.47
22	D	4031	CN3	OA-CB	2.33	1.50	1.43
16	C	4001	HEM	FE-NA	2.32	2.02	1.95
18	N	4110	8PE	O32-C31	-2.32	1.15	1.22
14	L	4113	6PH	C3-C2	2.31	1.58	1.50
22	N	4131	CN3	O41-C3'	-2.28	1.40	1.45
17	N	4025	SMA	C20-C19	2.25	1.35	1.33
22	N	4131	CN3	OA-CB	2.24	1.49	1.43
14	A	4013	6PH	C1-C2	2.24	1.57	1.50
18	C	4010	8PE	O32-C31	-2.20	1.15	1.22
20	C	4033	CN5	P'-O1'	2.18	1.67	1.59
16	D	4003	HEM	FE-NC	2.17	2.02	1.95
14	A	4013	6PH	C3-C2	2.16	1.57	1.50
16	C	4002	HEM	FE-NB	2.16	2.01	1.94
16	N	4021	HEM	CMC-C2C	2.14	1.55	1.50
20	C	4033	CN5	C42-C41	2.14	1.56	1.49
18	N	4110	8PE	C1-C2	2.12	1.57	1.50
16	C	4002	HEM	CMC-C2C	2.11	1.55	1.50
20	C	4033	CN5	C2'-C3'	-2.11	1.42	1.51
16	N	4022	HEM	CAC-C3C	-2.11	1.41	1.47
16	C	4002	HEM	FE-ND	2.09	2.01	1.94
20	C	4033	CN5	O31-C3	-2.07	1.39	1.45
16	C	4002	HEM	CAB-C3B	-2.06	1.41	1.47
20	C	4033	CN5	P'-O4'	2.04	1.64	1.55
14	A	4013	6PH	P-O11	-2.03	1.53	1.60
16	N	4021	HEM	CMA-C3A	2.02	1.54	1.50

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	4021	UMQ	CA-O1'-C1'	-8.62	98.95	113.68
15	L	4121	UMQ	CA-O1'-C1'	-8.34	99.44	113.68
20	C	4033	CN5	O1'-C1'-C2'	5.93	130.30	109.28
22	D	4031	CN3	C2'-O51-C51	-5.34	105.03	117.80
22	N	4131	CN3	C2'-O51-C51	-5.09	105.60	117.80
20	C	4033	CN5	C3'-C2'-C1'	-4.95	97.68	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	4033	CN5	P'-O1'-C1'	-4.26	100.98	121.26
14	L	4113	6PH	C3-C2-C1	-4.06	102.31	111.78
14	A	4013	6PH	C3-C2-C1	-4.04	102.36	111.78
15	L	4121	UMQ	O1'-CA-CB	3.93	122.69	109.37
19	N	4111	9PE	C2-O21-C21	-3.90	108.47	117.80
22	N	4131	CN3	C2-O21-C21	-3.89	108.50	117.80
20	C	4033	CN5	O11-C1-C2	-3.88	95.52	109.28
22	D	4031	CN3	C2-O21-C21	-3.72	108.89	117.80
15	A	4021	UMQ	O1'-CA-CB	3.69	121.89	109.37
19	C	4011	9PE	C2-O21-C21	-3.66	109.04	117.80
21	D	4014	7PH	C38-C37-C36	-3.63	96.04	114.37
21	O	4114	7PH	C38-C37-C36	-3.59	96.23	114.37
22	D	4031	CN3	C3-C2-C1	-3.58	103.44	111.78
18	C	4010	8PE	C2-O21-C21	-3.56	109.29	117.80
14	A	4013	6PH	O11-P-O12	3.54	116.01	106.44
18	C	4010	8PE	C3-C2-C1	3.52	119.99	111.78
14	L	4113	6PH	O11-P-O12	3.50	115.89	106.44
21	O	4114	7PH	O12-P-O11	3.48	115.75	106.67
21	D	4014	7PH	O12-P-O11	3.45	115.68	106.67
18	N	4110	8PE	C2-O21-C21	-3.45	109.54	117.80
22	N	4131	CN3	C3-C2-C1	-3.44	103.77	111.78
16	O	4023	HEM	CBB-CAB-C3B	-3.39	110.57	127.53
14	L	4113	6PH	O13-P-O11	3.23	115.10	106.67
22	D	4031	CN3	P-O13-CC	3.22	139.82	121.35
18	N	4110	8PE	C3-C2-C1	3.16	119.14	111.78
16	O	4023	HEM	CBC-CAC-C3C	-3.13	111.90	127.53
22	N	4131	CN3	P-O13-CC	3.10	139.12	121.35
16	D	4003	HEM	CBC-CAC-C3C	-3.09	112.07	127.53
14	A	4013	6PH	O13-P-O11	3.07	114.67	106.67
21	D	4014	7PH	C3-C2-C1	-3.02	104.74	111.78
22	D	4031	CN3	C3'-C2'-C1'	-3.02	104.75	111.78
21	D	4014	7PH	O13-P-O11	2.97	114.42	106.67
16	W	4026	HEM	CBB-CAB-C3B	-2.96	112.73	127.53
16	W	4026	HEM	CAC-C3C-C4C	-2.95	117.77	124.82
21	O	4114	7PH	O13-P-O11	2.95	114.36	106.67
16	D	4003	HEM	CBB-CAB-C3B	-2.91	112.99	127.53
21	O	4114	7PH	C3-C2-C1	-2.90	105.03	111.78
17	C	4005	SMA	C4A-C4-C3	-2.84	114.60	118.78
20	C	4033	CN5	P-O13-CC	2.81	137.44	121.35
17	N	4025	SMA	C4A-C4-C3	-2.72	114.77	118.78
16	W	4026	HEM	CBC-CAC-C3C	-2.69	114.09	127.53
22	N	4131	CN3	O4'-P'-O3'	2.67	119.69	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	4131	CN3	P-O11-C1	-2.66	106.11	121.35
14	L	4113	6PH	O14-P-O11	-2.64	99.78	106.67
22	D	4031	CN3	P-O11-C1	-2.61	106.39	121.35
17	N	4025	SMA	C9-C10-C11	-2.59	109.61	114.46
16	N	4021	HEM	CAD-C3D-C4D	2.58	129.19	124.70
15	L	4121	UMQ	C3'-C4'-C5'	-2.51	105.37	110.93
16	N	4021	HEM	CAC-C3C-C4C	2.50	130.80	124.82
15	A	4021	UMQ	CD-CC-CB	-2.49	101.79	114.37
22	D	4031	CN3	O4'-P'-O3'	2.48	118.79	107.57
22	N	4131	CN3	C3'-C2'-C1'	-2.47	106.02	111.78
21	D	4014	7PH	O11-P-O14	-2.47	99.76	106.44
20	C	4033	CN5	C3-C2-C1	-2.45	105.76	113.67
16	C	4001	HEM	CAC-C3C-C4C	2.45	130.66	124.82
14	A	4013	6PH	O14-P-O11	-2.45	100.29	106.67
15	A	4021	UMQ	O1-C1-O5	-2.44	104.27	110.69
20	C	4033	CN5	C33-C32-C31	2.43	122.59	113.69
16	C	4001	HEM	CAD-C3D-C4D	2.42	128.91	124.70
15	A	4021	UMQ	C3'-C4'-C5'	-2.41	105.59	110.93
15	L	4121	UMQ	CD-CC-CB	-2.39	102.29	114.37
17	C	4005	SMA	O1-C2-C3	2.33	123.87	121.81
21	O	4114	7PH	O11-P-O14	-2.33	100.14	106.44
16	D	4003	HEM	CAC-C3C-C4C	-2.30	119.33	124.82
21	O	4114	7PH	O31-C31-C32	-2.29	104.84	111.83
21	O	4114	7PH	O31-C3-C2	-2.29	101.79	108.40
15	L	4121	UMQ	O1'-C1'-C2'	2.27	111.71	108.27
16	N	4021	HEM	CAD-C3D-C2D	-2.26	123.63	127.87
17	N	4025	SMA	O8-C8-C7	2.26	124.07	119.21
21	D	4014	7PH	O31-C31-C32	-2.23	105.04	111.83
21	D	4014	7PH	O31-C31-O32	2.21	129.15	123.63
21	O	4114	7PH	O31-C31-O32	2.21	129.15	123.63
15	A	4021	UMQ	O1'-C1'-C2'	2.20	111.61	108.27
16	C	4001	HEM	CBC-CAC-C3C	-2.19	116.57	127.53
17	C	4005	SMA	C9-C10-C11	-2.17	110.41	114.46
22	D	4031	CN3	O4'-P'-O2'	-2.14	102.47	112.44
21	D	4014	7PH	O31-C3-C2	-2.11	102.32	108.40
16	W	4026	HEM	CAD-C3D-C4D	2.10	128.36	124.70
16	C	4001	HEM	CAD-C3D-C2D	-2.10	123.94	127.87
15	L	4121	UMQ	O1-C1-O5	-2.09	105.19	110.69
20	C	4033	CN5	C36-C35-C34	2.07	124.85	114.37
17	C	4005	SMA	O8-C8-C7	2.07	123.66	119.21
16	W	4026	HEM	CAC-C3C-C2C	2.06	135.12	128.43
15	L	4121	UMQ	CC-CB-CA	2.04	122.34	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	4021	UMQ	C1-O5-C5	-2.04	109.74	113.72
20	C	4033	CN5	P-O11-C1	-2.03	111.58	121.26
22	N	4131	CN3	P'-O3'-CA	2.01	132.89	121.35
22	D	4031	CN3	CC-CB-CA	-2.01	106.87	112.65
22	N	4131	CN3	O4'-P'-O2'	-2.00	103.14	112.44

There are no chirality outliers.

All (263) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	C	4011	9PE	C1-O11-P-O12
19	C	4011	9PE	C1-O11-P-O13
19	C	4011	9PE	C1-O11-P-O14
19	C	4011	9PE	C11-O13-P-O11
19	C	4011	9PE	C11-O13-P-O14
19	N	4111	9PE	C1-O11-P-O12
19	N	4111	9PE	C1-O11-P-O13
19	N	4111	9PE	C1-O11-P-O14
19	N	4111	9PE	O13-C11-C12-N
20	C	4033	CN5	CB-CC-O13-P
22	D	4031	CN3	C1-O11-P-O14
22	D	4031	CN3	CC-O13-P-O11
22	D	4031	CN3	CC-O13-P-O12
22	D	4031	CN3	CC-O13-P-O14
22	D	4031	CN3	O11-C1-C2-O21
22	D	4031	CN3	C22-C21-O21-C2
22	D	4031	CN3	CA-O3'-P'-O1'
22	D	4031	CN3	O1'-C1'-C2'-O51
22	D	4031	CN3	C52-C51-O51-C2'
22	N	4131	CN3	C1-O11-P-O14
22	N	4131	CN3	CC-O13-P-O11
22	N	4131	CN3	CC-O13-P-O12
22	N	4131	CN3	CC-O13-P-O14
22	N	4131	CN3	O11-C1-C2-O21
22	N	4131	CN3	C22-C21-O21-C2
22	N	4131	CN3	CA-O3'-P'-O1'
22	N	4131	CN3	O1'-C1'-C2'-O51
22	N	4131	CN3	C52-C51-O51-C2'
22	D	4031	CN3	O32-C31-O31-C3
22	D	4031	CN3	O22-C21-O21-C2
22	D	4031	CN3	O52-C51-O51-C2'
22	N	4131	CN3	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
22	N	4131	CN3	O52-C51-O51-C2'
22	D	4031	CN3	C32-C31-O31-C3
20	C	4033	CN5	C32-C31-O31-C3
22	N	4131	CN3	C32-C31-O31-C3
22	N	4131	CN3	O32-C31-O31-C3
20	C	4033	CN5	O3'-CA-CB-OA
20	C	4033	CN5	O32-C31-O31-C3
15	A	4021	UMQ	O1'-CA-CB-CC
15	L	4121	UMQ	O1'-CA-CB-CC
20	C	4033	CN5	O3'-CA-CB-CC
18	N	4110	8PE	C21-C22-C23-C24
22	D	4031	CN3	C43-C44-C45-C46
18	C	4010	8PE	C21-C22-C23-C24
21	O	4114	7PH	C31-C32-C33-C34
22	D	4031	CN3	O3'-CA-CB-OA
22	N	4131	CN3	O3'-CA-CB-OA
21	D	4014	7PH	C21-C22-C23-C24
14	L	4113	6PH	C22-C21-O21-C2
22	N	4131	CN3	C41-C42-C43-C44
14	L	4113	6PH	O22-C21-O21-C2
22	D	4031	CN3	O3'-CA-CB-CC
22	N	4131	CN3	O3'-CA-CB-CC
21	D	4014	7PH	C31-C32-C33-C34
14	L	4113	6PH	C37-C38-C39-C3A
18	N	4110	8PE	C32-C33-C34-C35
18	N	4110	8PE	C36-C37-C38-C39
19	C	4011	9PE	C2E-C2F-C2G-C2H
20	C	4033	CN5	C3A-C3B-C3C-C3D
22	D	4031	CN3	C52-C53-C54-C55
14	A	4013	6PH	C27-C28-C29-C2A
18	N	4110	8PE	C3A-C3B-C3C-C3D
18	C	4010	8PE	C37-C38-C39-C3A
21	D	4014	7PH	C32-C33-C34-C35
19	N	4111	9PE	C2C-C2D-C2E-C2F
21	O	4114	7PH	C27-C28-C29-C2A
18	C	4010	8PE	O11-C1-C2-C3
18	N	4110	8PE	O11-C1-C2-C3
21	D	4014	7PH	C37-C38-C39-C3A
22	N	4131	CN3	C55-C56-C57-C58
19	N	4111	9PE	C2E-C2F-C2G-C2H
20	C	4033	CN5	C37-C38-C39-C3A
21	D	4014	7PH	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
19	C	4011	9PE	C26-C27-C28-C29
21	O	4114	7PH	C32-C33-C34-C35
14	L	4113	6PH	C32-C33-C34-C35
20	C	4033	CN5	C3B-C3C-C3D-C3E
20	C	4033	CN5	C39-C3A-C3B-C3C
22	D	4031	CN3	C53-C54-C55-C56
14	A	4013	6PH	C39-C3A-C3B-C3C
18	N	4110	8PE	C2A-C2B-C2C-C2D
22	N	4131	CN3	C46-C47-C48-C49
15	A	4021	UMQ	CF-CG-CH-CI
18	N	4110	8PE	C33-C34-C35-C36
21	O	4114	7PH	C37-C38-C39-C3A
15	L	4121	UMQ	CD-CF-CG-CH
18	N	4110	8PE	C35-C36-C37-C38
20	C	4033	CN5	C42-C41-O41-C3'
14	L	4113	6PH	C36-C37-C38-C39
21	D	4014	7PH	C2A-C2B-C2C-C2D
22	D	4031	CN3	C42-C43-C44-C45
14	A	4013	6PH	C22-C21-O21-C2
14	A	4013	6PH	O22-C21-O21-C2
16	D	4003	HEM	C2C-C3C-CAC-CBC
19	N	4111	9PE	C26-C27-C28-C29
19	C	4011	9PE	C22-C23-C24-C25
21	O	4114	7PH	C26-C27-C28-C29
18	N	4110	8PE	C31-C32-C33-C34
19	N	4111	9PE	C28-C29-C2A-C2B
21	D	4014	7PH	C27-C28-C29-C2A
14	L	4113	6PH	C35-C36-C37-C38
18	N	4110	8PE	C3C-C3D-C3E-C3F
19	C	4011	9PE	C2D-C2E-C2F-C2G
14	L	4113	6PH	C38-C39-C3A-C3B
14	A	4013	6PH	C34-C35-C36-C37
19	C	4011	9PE	C28-C29-C2A-C2B
21	O	4114	7PH	C22-C23-C24-C25
18	C	4010	8PE	C29-C2A-C2B-C2C
19	C	4011	9PE	O11-C1-C2-C3
19	N	4111	9PE	O11-C1-C2-C3
22	D	4031	CN3	O11-C1-C2-C3
22	D	4031	CN3	O1'-C1'-C2'-C3'
22	N	4131	CN3	O11-C1-C2-C3
22	N	4131	CN3	O1'-C1'-C2'-C3'
14	A	4013	6PH	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
14	A	4013	6PH	C35-C36-C37-C38
18	C	4010	8PE	C32-C33-C34-C35
18	C	4010	8PE	C3B-C3C-C3D-C3E
19	N	4111	9PE	C22-C23-C24-C25
20	C	4033	CN5	O11-C1-C2-C3
20	C	4033	CN5	O1'-C1'-C2'-C3'
14	A	4013	6PH	C29-C2A-C2B-C2C
14	A	4013	6PH	C2B-C2C-C2D-C2E
18	N	4110	8PE	C26-C27-C28-C29
14	A	4013	6PH	C25-C26-C27-C28
18	N	4110	8PE	C3B-C3C-C3D-C3E
18	N	4110	8PE	C23-C24-C25-C26
14	L	4113	6PH	C29-C2A-C2B-C2C
17	C	4005	SMA	C9-C10-C11-C22
14	L	4113	6PH	C28-C29-C2A-C2B
15	L	4121	UMQ	CF-CG-CH-CI
22	N	4131	CN3	C47-C48-C49-C4A
18	N	4110	8PE	C38-C39-C3A-C3B
19	N	4111	9PE	C29-C2A-C2B-C2C
21	D	4014	7PH	C26-C27-C28-C29
19	N	4111	9PE	C2A-C2B-C2C-C2D
19	N	4111	9PE	C21-C22-C23-C24
21	D	4014	7PH	C2B-C2C-C2D-C2E
14	L	4113	6PH	C27-C28-C29-C2A
22	D	4031	CN3	C21-C22-C23-C24
22	N	4131	CN3	C21-C22-C23-C24
20	C	4033	CN5	C38-C39-C3A-C3B
15	A	4021	UMQ	CI-CJ-CK-CL
21	O	4114	7PH	C2A-C2B-C2C-C2D
14	A	4013	6PH	C32-C33-C34-C35
18	C	4010	8PE	C35-C36-C37-C38
20	C	4033	CN5	C35-C36-C37-C38
15	A	4021	UMQ	CD-CF-CG-CH
19	C	4011	9PE	O11-C1-C2-O21
19	N	4111	9PE	O11-C1-C2-O21
14	A	4013	6PH	C36-C37-C38-C39
18	C	4010	8PE	C34-C35-C36-C37
22	N	4131	CN3	C56-C57-C58-C59
18	C	4010	8PE	C33-C34-C35-C36
19	C	4011	9PE	C24-C25-C26-C27
22	D	4031	CN3	C47-C48-C49-C4A
15	L	4121	UMQ	CG-CH-CI-CJ

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Mol	Chain	Res	Type	Atoms
14	L	4113	6PH	C34-C35-C36-C37
20	C	4033	CN5	O42-C41-O41-C3'
18	C	4010	8PE	C28-C29-C2A-C2B
22	D	4031	CN3	C45-C46-C47-C48
19	C	4011	9PE	O31-C31-C32-C33
21	D	4014	7PH	C36-C37-C38-C39
19	N	4111	9PE	C24-C25-C26-C27
16	D	4003	HEM	C2B-C3B-CAB-CBB
16	O	4023	HEM	C2B-C3B-CAB-CBB
16	O	4023	HEM	C2C-C3C-CAC-CBC
16	W	4026	HEM	C2B-C3B-CAB-CBB
16	W	4026	HEM	C2C-C3C-CAC-CBC
14	L	4113	6PH	O11-C1-C2-O21
18	C	4010	8PE	O11-C1-C2-O21
18	N	4110	8PE	O11-C1-C2-O21
18	N	4110	8PE	C29-C2A-C2B-C2C
21	O	4114	7PH	C22-C21-O21-C2
18	C	4010	8PE	C2A-C2B-C2C-C2D
18	C	4010	8PE	C36-C37-C38-C39
18	C	4010	8PE	C3A-C3B-C3C-C3D
14	A	4013	6PH	O11-C1-C2-C3
14	L	4113	6PH	O11-C1-C2-C3
21	O	4114	7PH	O22-C21-O21-C2
18	N	4110	8PE	C3D-C3E-C3F-C3G
22	N	4131	CN3	C44-C45-C46-C47
19	C	4011	9PE	C11-O13-P-O12
20	C	4033	CN5	C1-O11-P-O14
22	D	4031	CN3	CA-O3'-P'-O2'
22	N	4131	CN3	CA-O3'-P'-O2'
20	C	4033	CN5	CB-CA-O3'-P'
22	D	4031	CN3	C46-C47-C48-C49
19	C	4011	9PE	C23-C24-C25-C26
14	L	4113	6PH	C2C-C2D-C2E-C2F
22	N	4131	CN3	C53-C54-C55-C56
19	N	4111	9PE	O31-C31-C32-C33
14	L	4113	6PH	C25-C26-C27-C28
17	C	4005	SMA	C6-C5-O5-C5M
20	C	4033	CN5	C31-C32-C33-C34
19	N	4111	9PE	C23-C24-C25-C26
16	O	4023	HEM	CAA-CBA-CGA-O2A
16	D	4003	HEM	C4B-C3B-CAB-CBB
16	D	4003	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
16	O	4023	HEM	C4B-C3B-CAB-CBB
18	C	4010	8PE	C3C-C3D-C3E-C3F
21	D	4014	7PH	C23-C24-C25-C26
17	C	4005	SMA	C4A-C5-O5-C5M
22	N	4131	CN3	C43-C44-C45-C46
16	C	4001	HEM	CAA-CBA-CGA-O2A
18	C	4010	8PE	C3E-C3F-C3G-C3H
16	O	4023	HEM	CAA-CBA-CGA-O1A
14	A	4013	6PH	C28-C29-C2A-C2B
16	C	4001	HEM	CAA-CBA-CGA-O1A
16	D	4003	HEM	CAA-CBA-CGA-O2A
16	C	4002	HEM	CAA-CBA-CGA-O2A
19	C	4011	9PE	C27-C28-C29-C2A
16	C	4002	HEM	CAA-CBA-CGA-O1A
16	D	4003	HEM	CAA-CBA-CGA-O1A
16	N	4021	HEM	CAA-CBA-CGA-O1A
16	N	4021	HEM	CAA-CBA-CGA-O2A
16	N	4022	HEM	CAA-CBA-CGA-O2A
16	N	4022	HEM	CAD-CBD-CGD-O2D
16	N	4022	HEM	CAD-CBD-CGD-O1D
21	O	4114	7PH	C34-C35-C36-C37
14	A	4013	6PH	C24-C25-C26-C27
22	D	4031	CN3	C41-C42-C43-C44
19	C	4011	9PE	C2B-C2C-C2D-C2E
14	L	4113	6PH	C3A-C3B-C3C-C3D
16	N	4022	HEM	CAA-CBA-CGA-O1A
16	C	4001	HEM	CAD-CBD-CGD-O2D
16	N	4021	HEM	CAD-CBD-CGD-O2D
21	O	4114	7PH	C38-C39-C3A-C3B
16	C	4002	HEM	CAD-CBD-CGD-O2D
16	C	4001	HEM	CAD-CBD-CGD-O1D
16	N	4021	HEM	C2B-C3B-CAB-CBB
21	O	4114	7PH	C21-C22-C23-C24
18	N	4110	8PE	C28-C29-C2A-C2B
14	L	4113	6PH	C33-C34-C35-C36
16	D	4003	HEM	CAD-CBD-CGD-O2D
19	C	4011	9PE	C21-C22-C23-C24
16	N	4021	HEM	C4B-C3B-CAB-CBB
16	O	4023	HEM	C4C-C3C-CAC-CBC
16	W	4026	HEM	C4B-C3B-CAB-CBB
16	W	4026	HEM	C4C-C3C-CAC-CBC
16	N	4021	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
16	C	4002	HEM	CAD-CBD-CGD-O1D
16	D	4003	HEM	CAD-CBD-CGD-O1D
14	A	4013	6PH	O31-C31-C32-C33
18	N	4110	8PE	C27-C28-C29-C2A
17	N	4025	SMA	C3-C2-C9-C10
18	N	4110	8PE	C37-C38-C39-C3A
22	N	4131	CN3	C48-C49-C4A-C4B
14	L	4113	6PH	O31-C31-C32-C33
21	D	4014	7PH	C33-C34-C35-C36
19	C	4011	9PE	O32-C31-C32-C33
22	D	4031	CN3	C54-C55-C56-C57
16	O	4023	HEM	CAD-CBD-CGD-O2D
14	L	4113	6PH	O32-C31-C32-C33
19	C	4011	9PE	C2C-C2D-C2E-C2F
14	A	4013	6PH	O32-C31-C32-C33
16	O	4023	HEM	CAD-CBD-CGD-O1D
18	N	4110	8PE	O31-C31-C32-C33
18	C	4010	8PE	C27-C28-C29-C2A
21	D	4014	7PH	C29-C2A-C2B-C2C
22	N	4131	CN3	C51-C52-C53-C54
16	W	4026	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

17 monomers are involved in 35 short contacts:

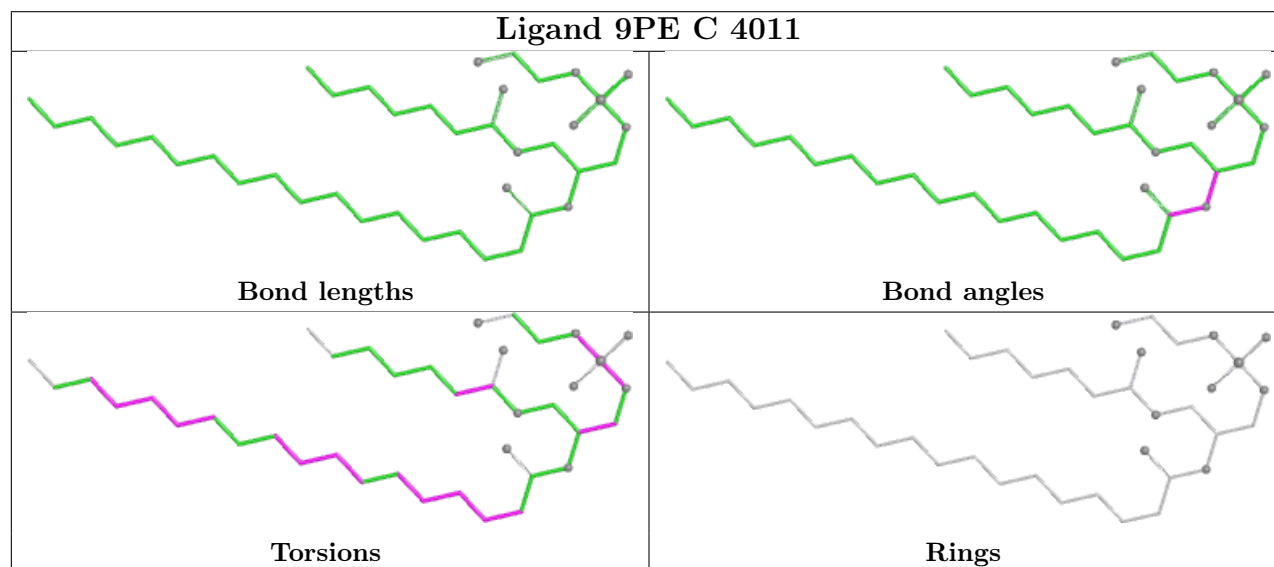
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	D	4031	CN3	5	0
21	D	4014	7PH	2	0
18	C	4010	8PE	1	0
14	L	4113	6PH	3	0
14	A	4013	6PH	1	0
16	D	4003	HEM	1	0
16	C	4001	HEM	1	0
16	N	4021	HEM	2	0
22	N	4131	CN3	5	0
16	C	4002	HEM	1	0
17	N	4025	SMA	1	0
15	A	4021	UMQ	2	0
16	N	4022	HEM	2	0
21	O	4114	7PH	2	0
20	C	4033	CN5	5	0
17	C	4005	SMA	2	0

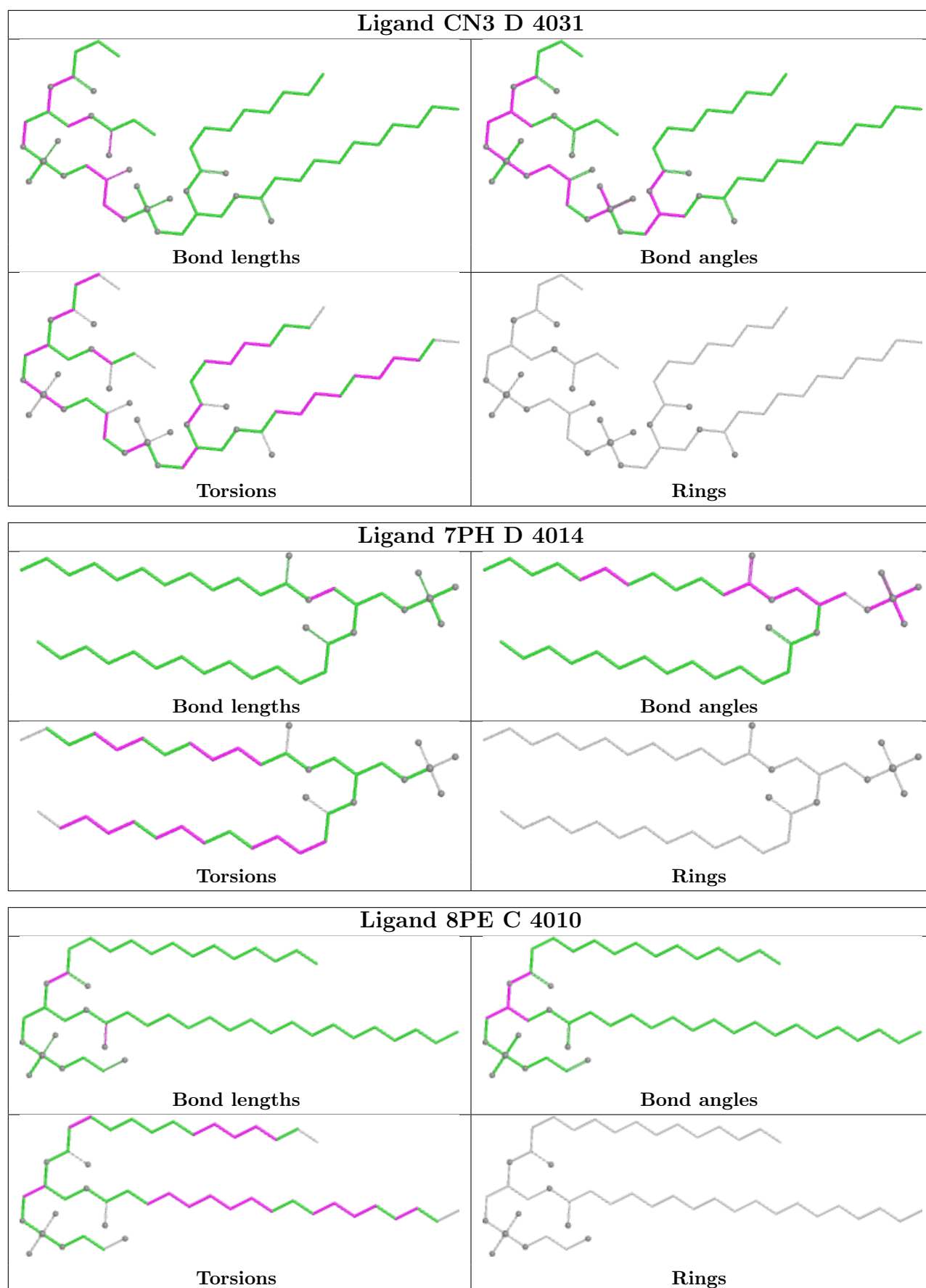
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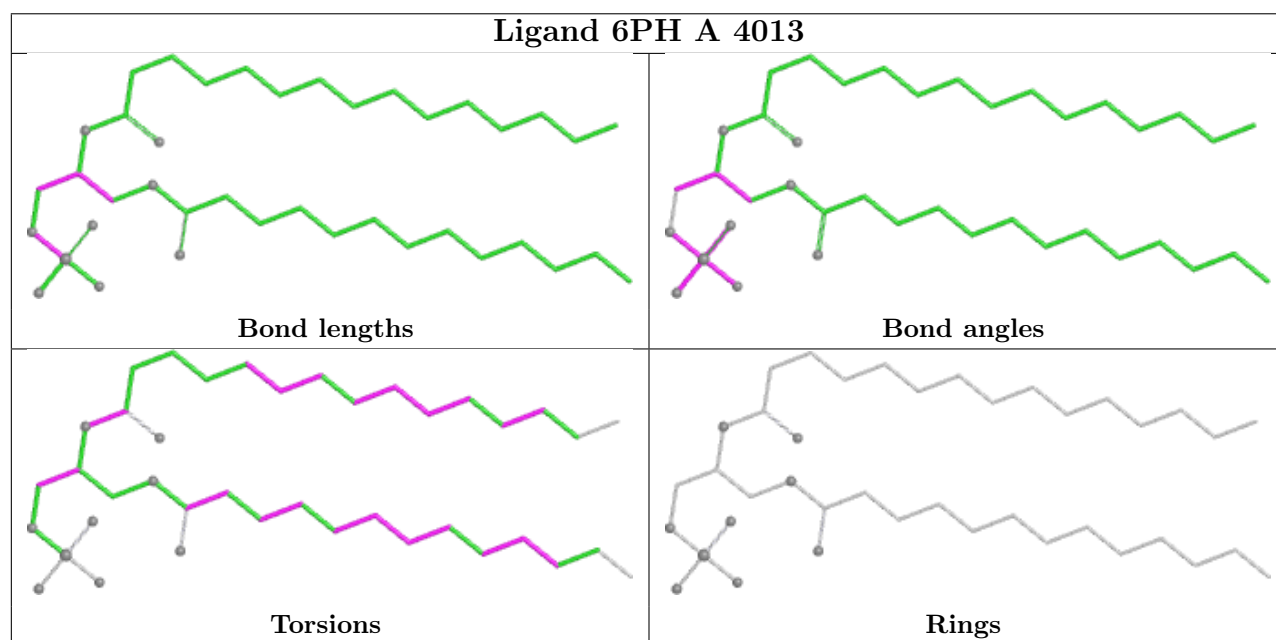
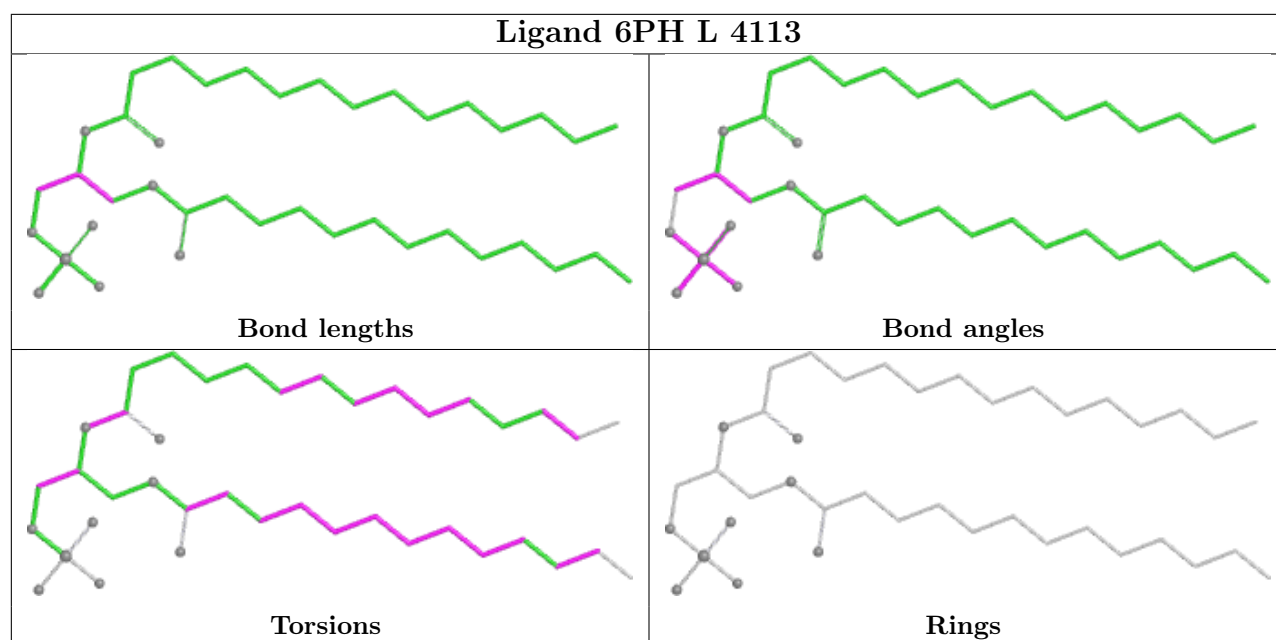
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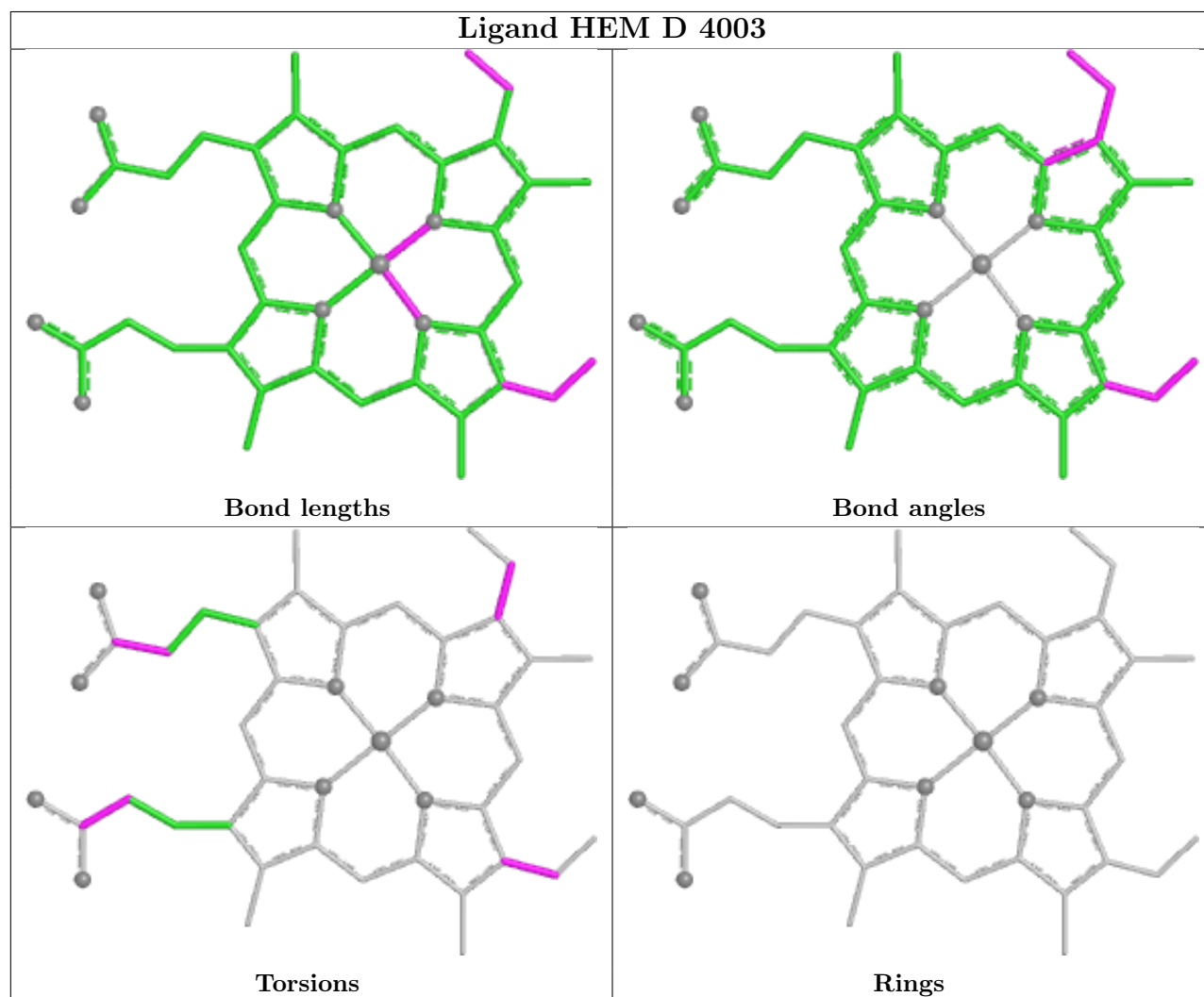
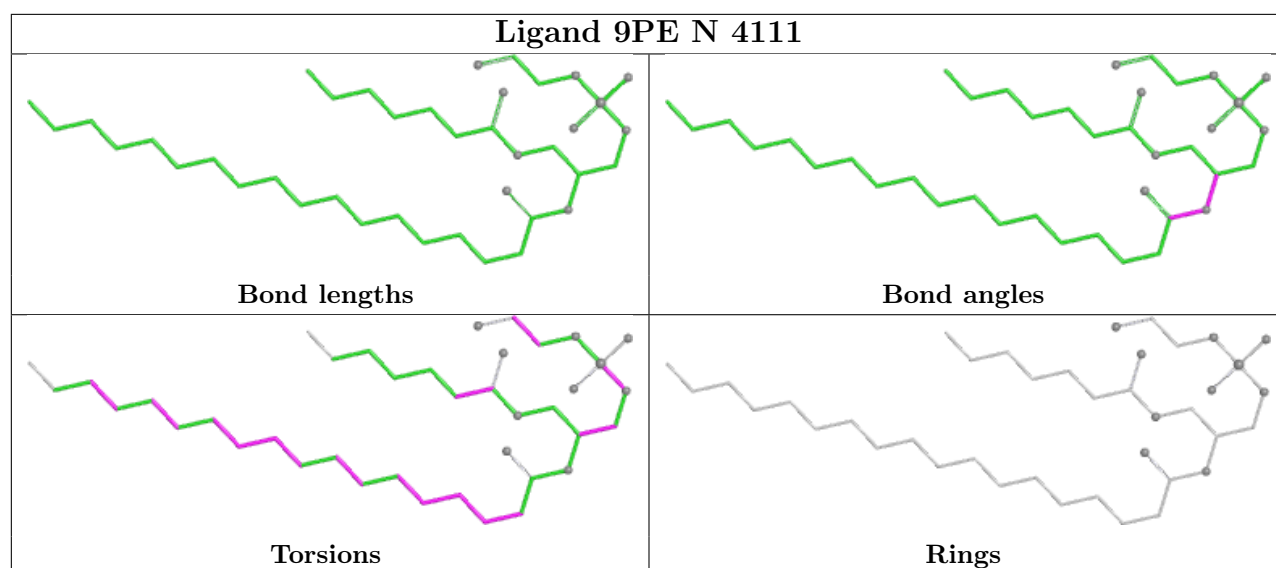
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	L	4121	UMQ	2	0

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

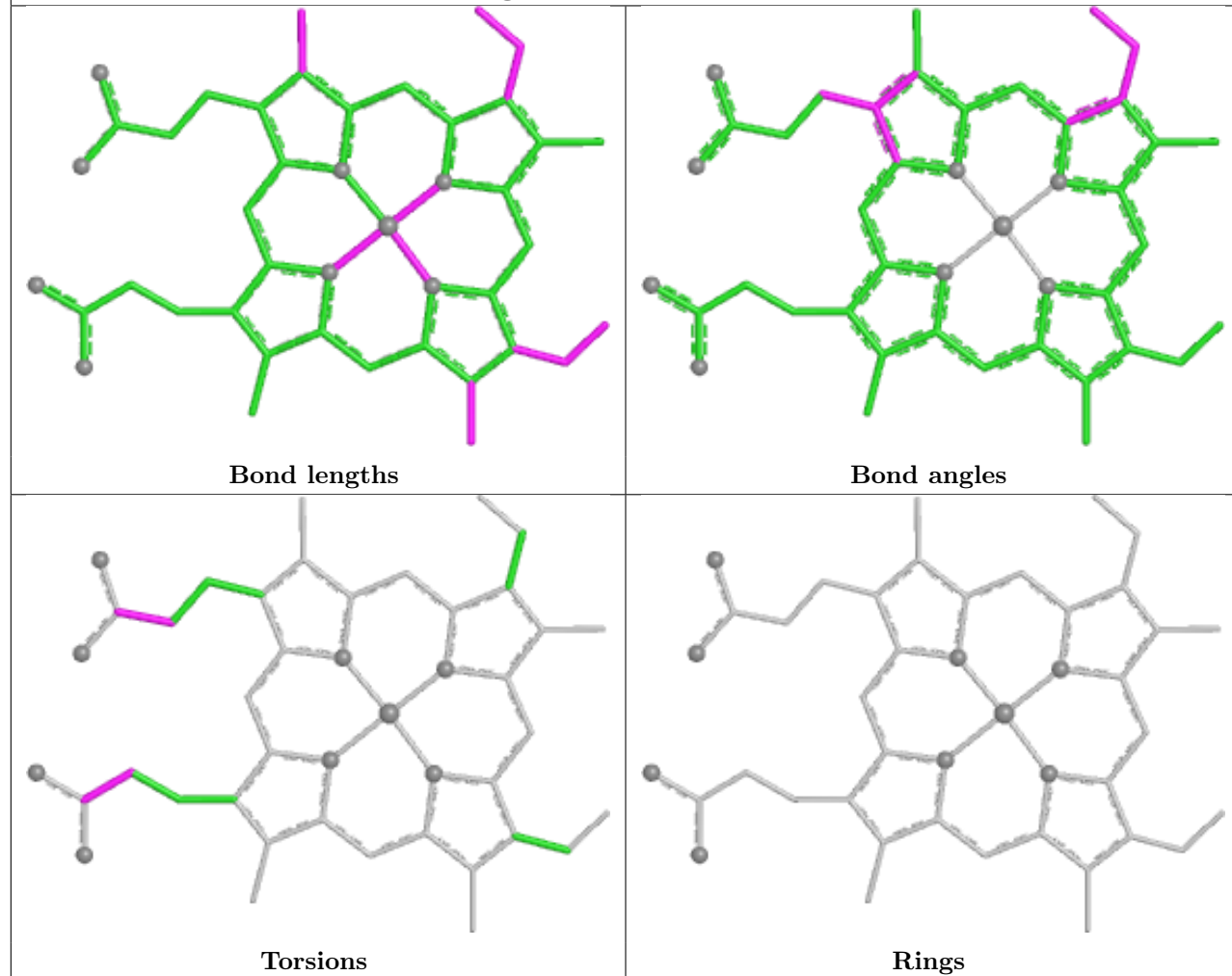




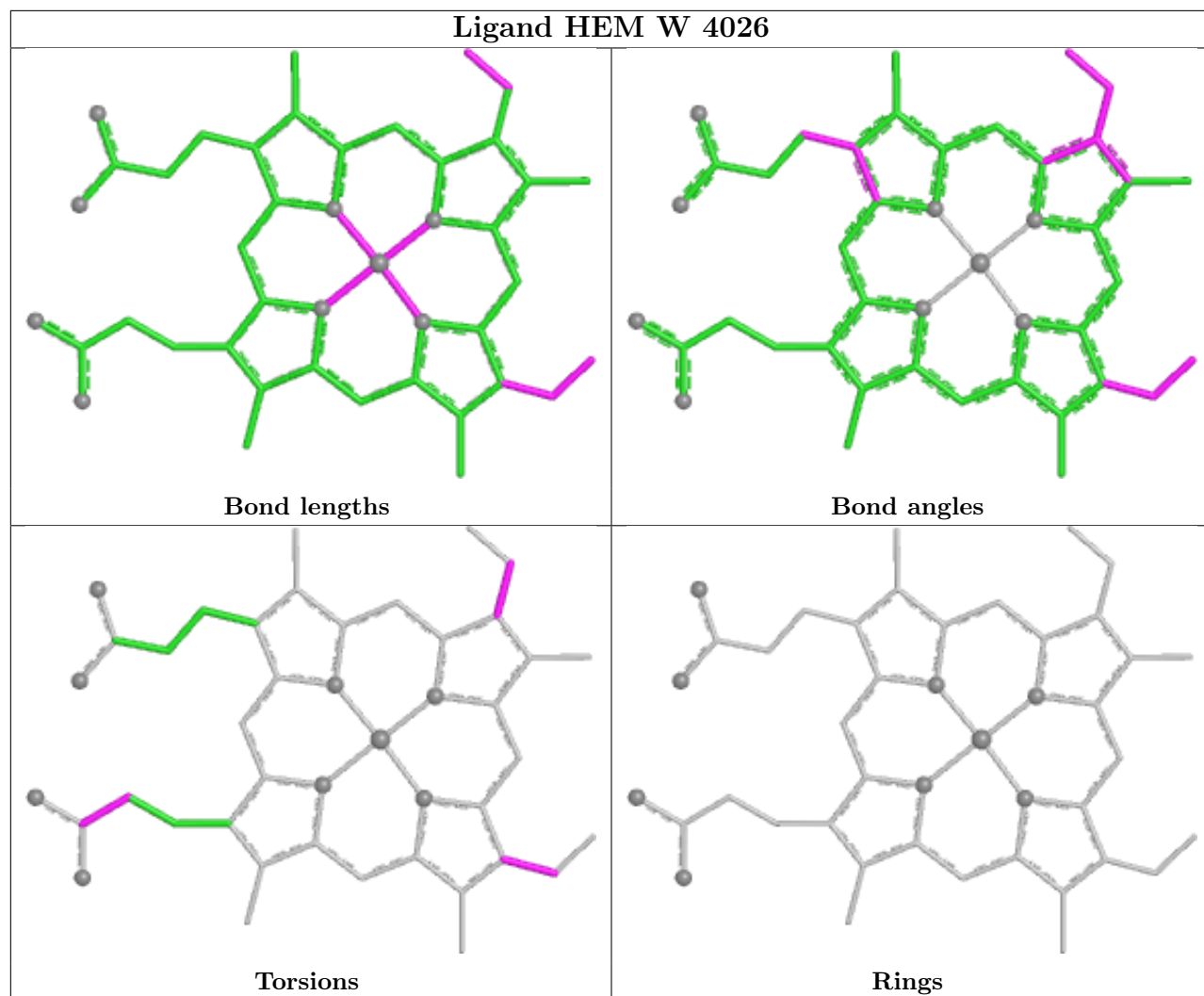




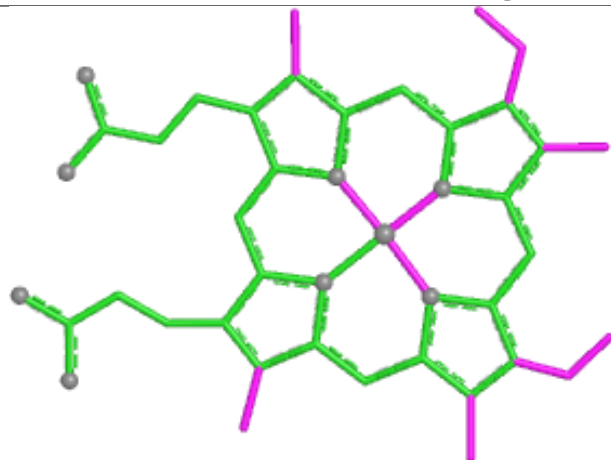
Ligand HEM C 4001



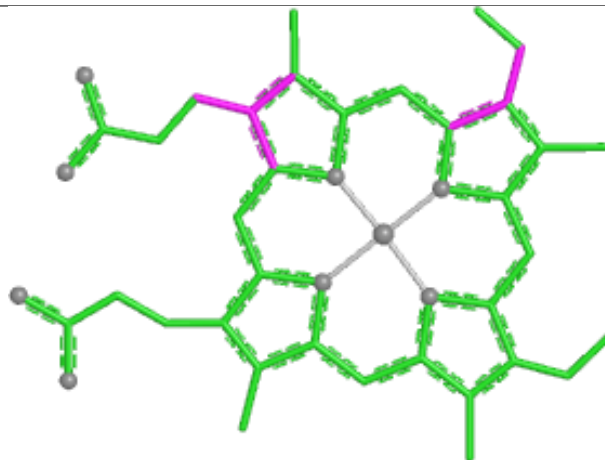
Ligand HEM W 4026



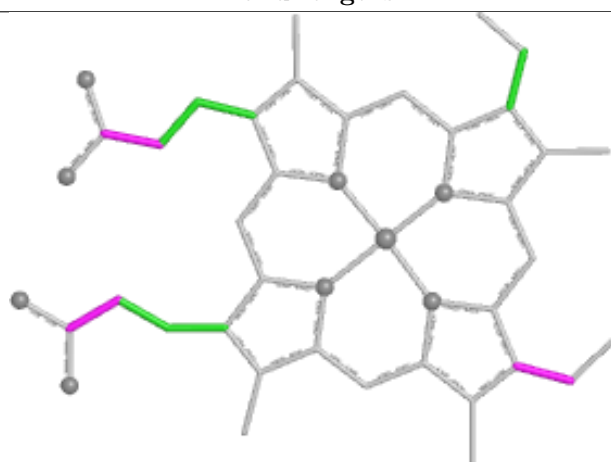
Ligand HEM N 4021



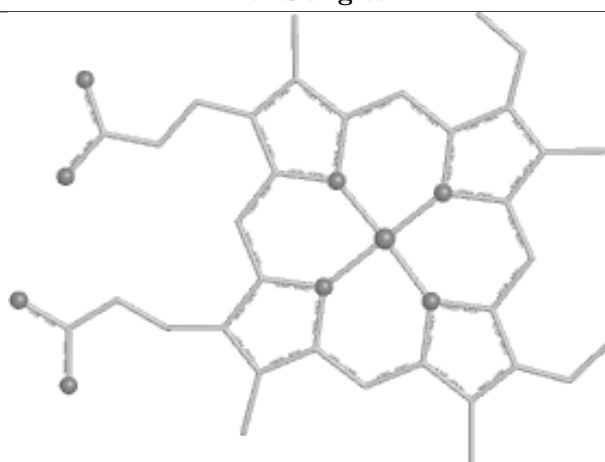
Bond lengths



Bond angles

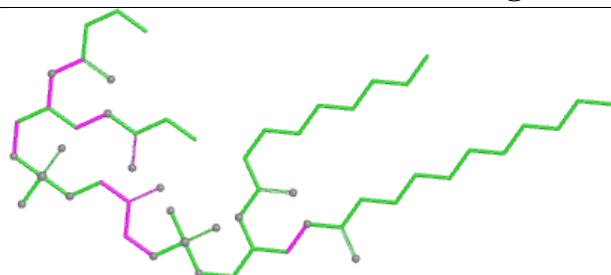


Torsions

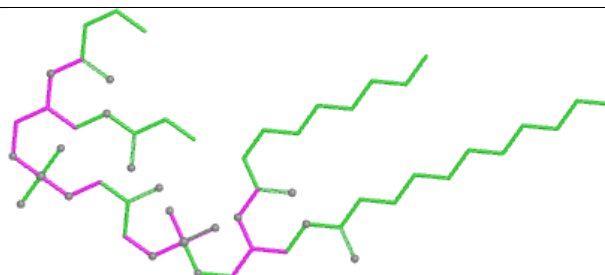


Rings

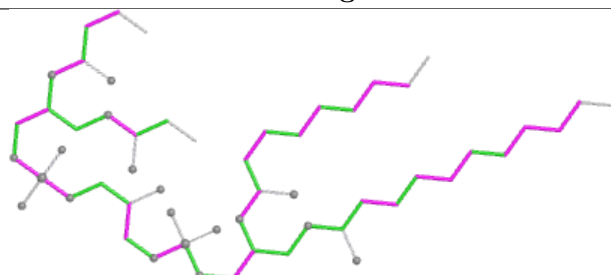
Ligand CN3 N 4131



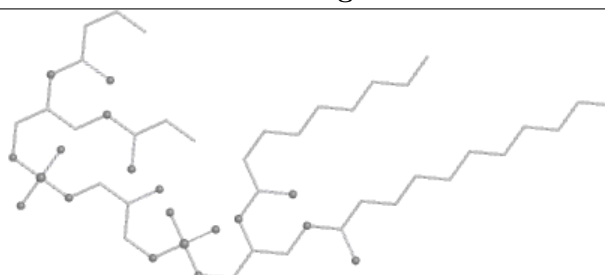
Bond lengths



Bond angles

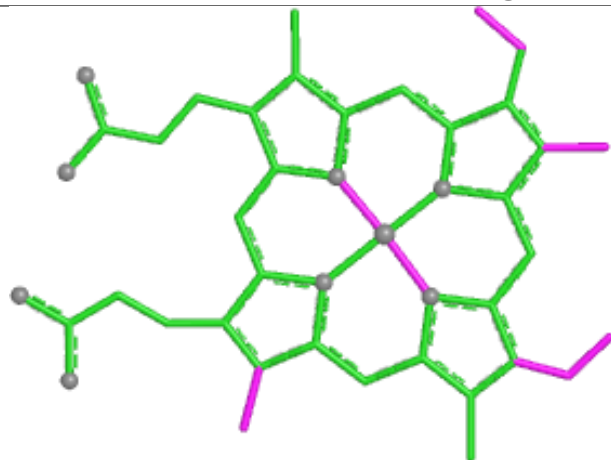


Torsions

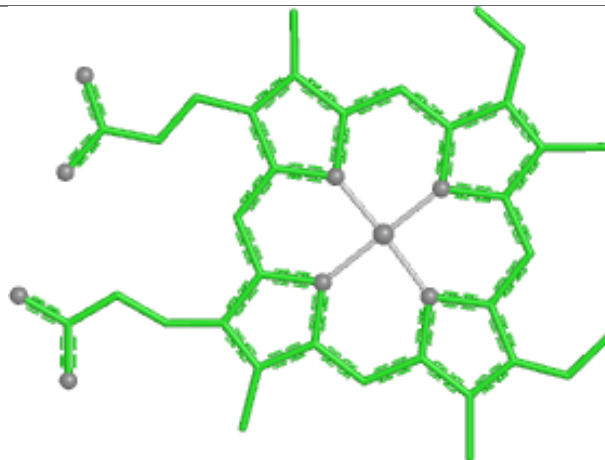


Rings

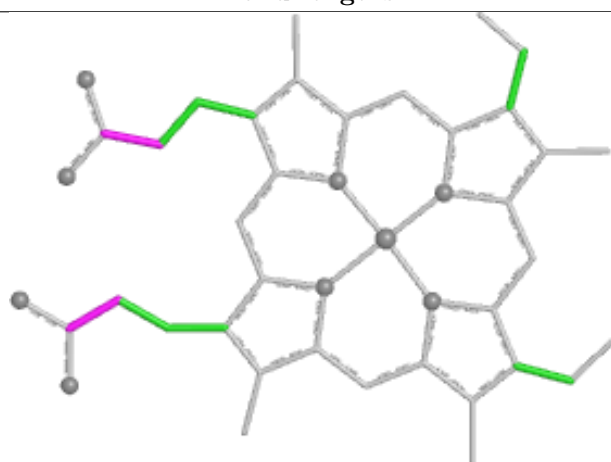
Ligand HEM C 4002



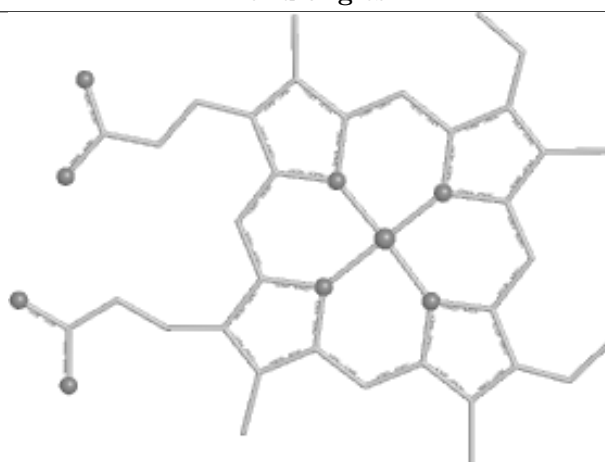
Bond lengths



Bond angles

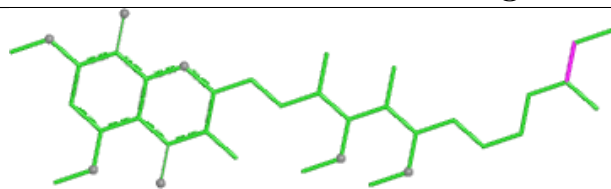


Torsions

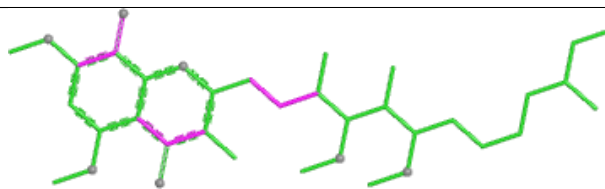


Rings

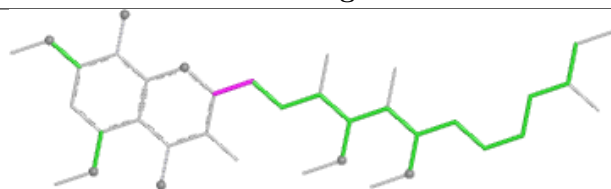
Ligand SMA N 4025



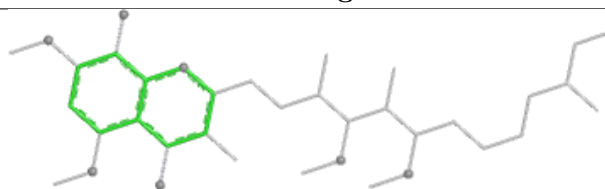
Bond lengths



Bond angles

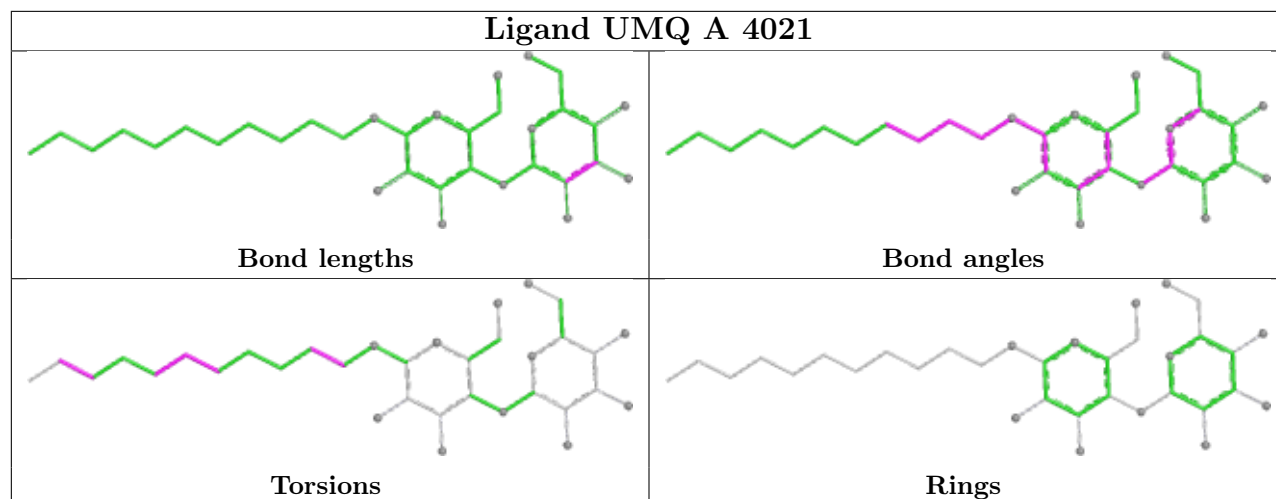


Torsions

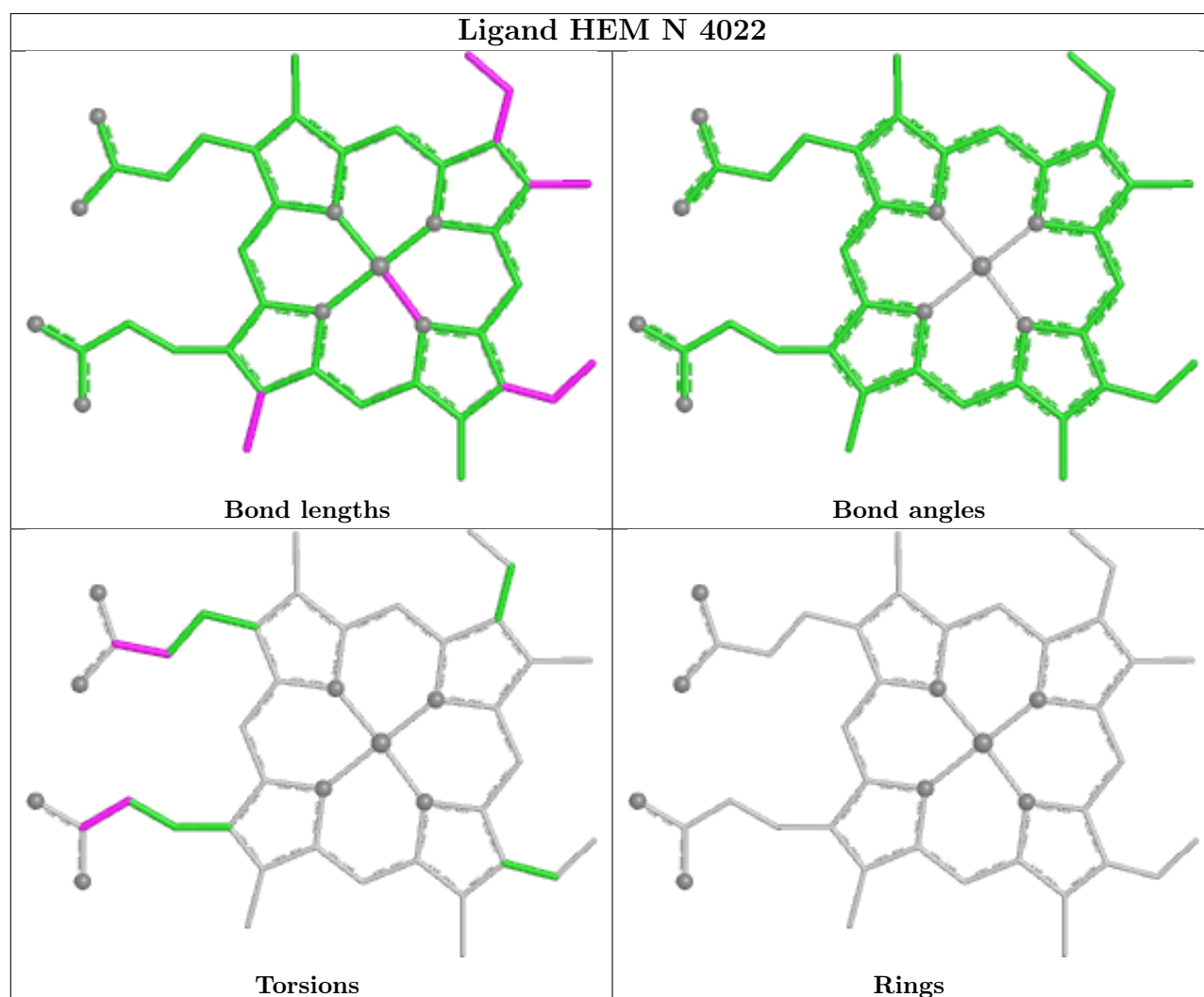


Rings

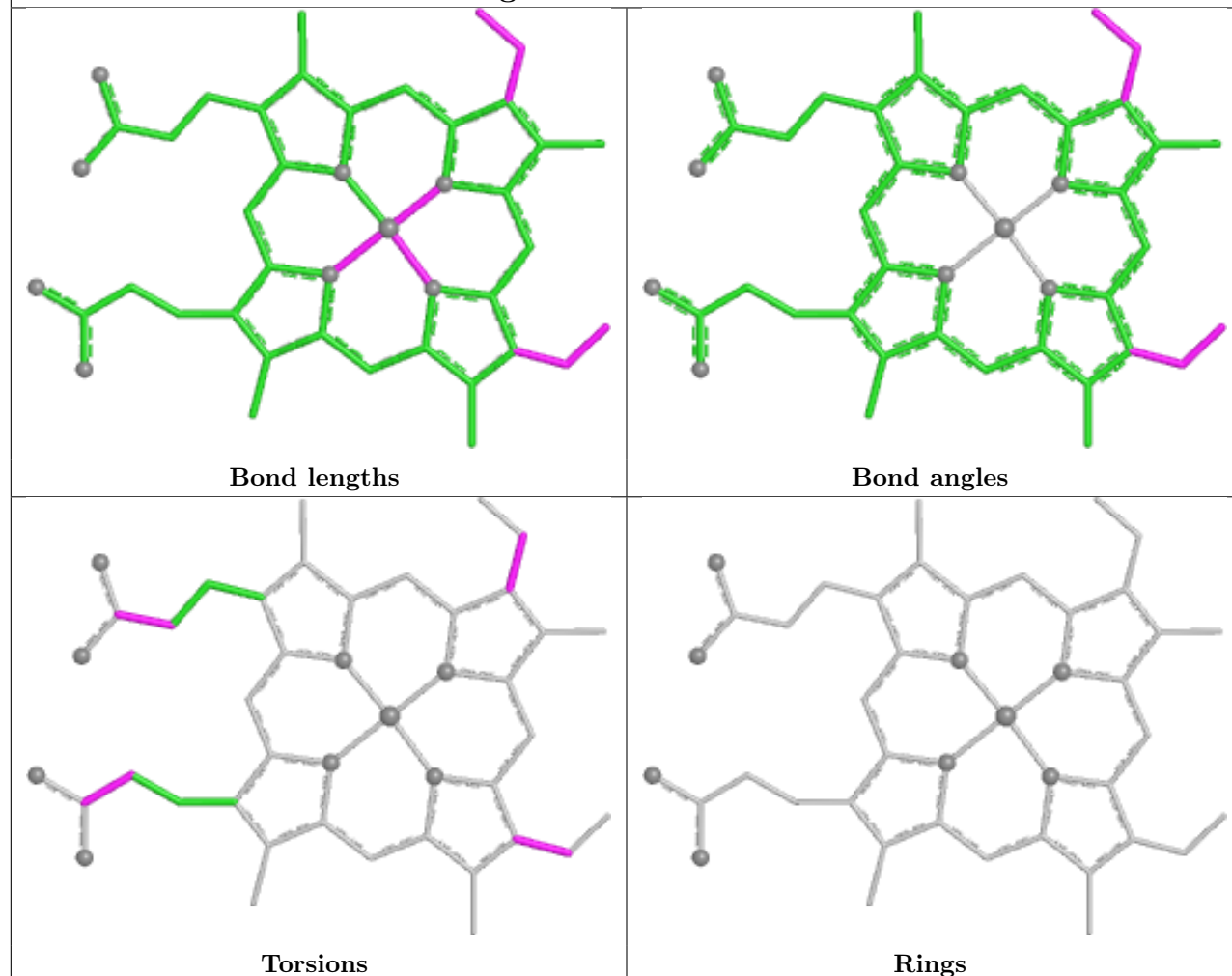
Ligand UMQ A 4021



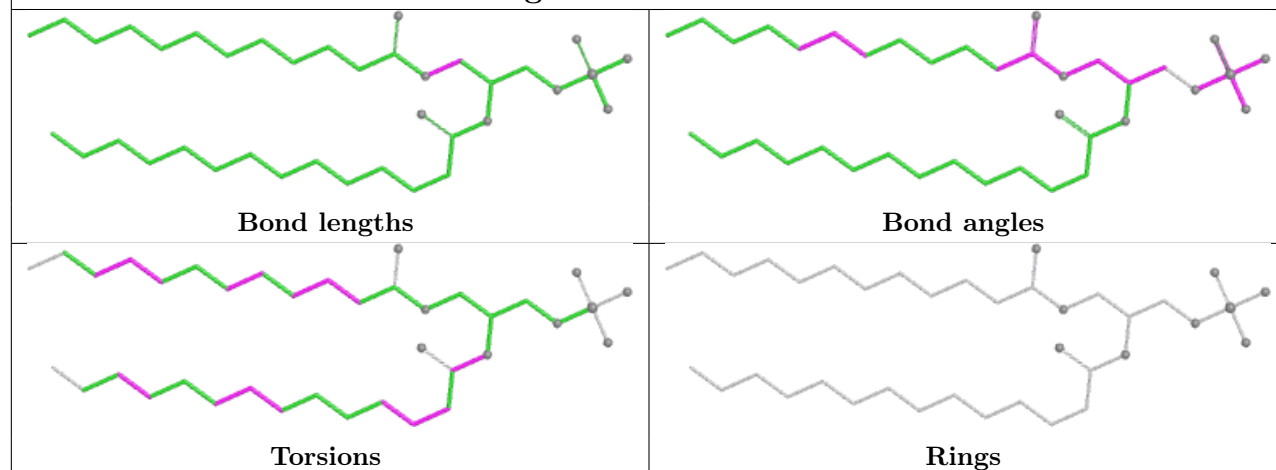
Ligand HEM N 4022

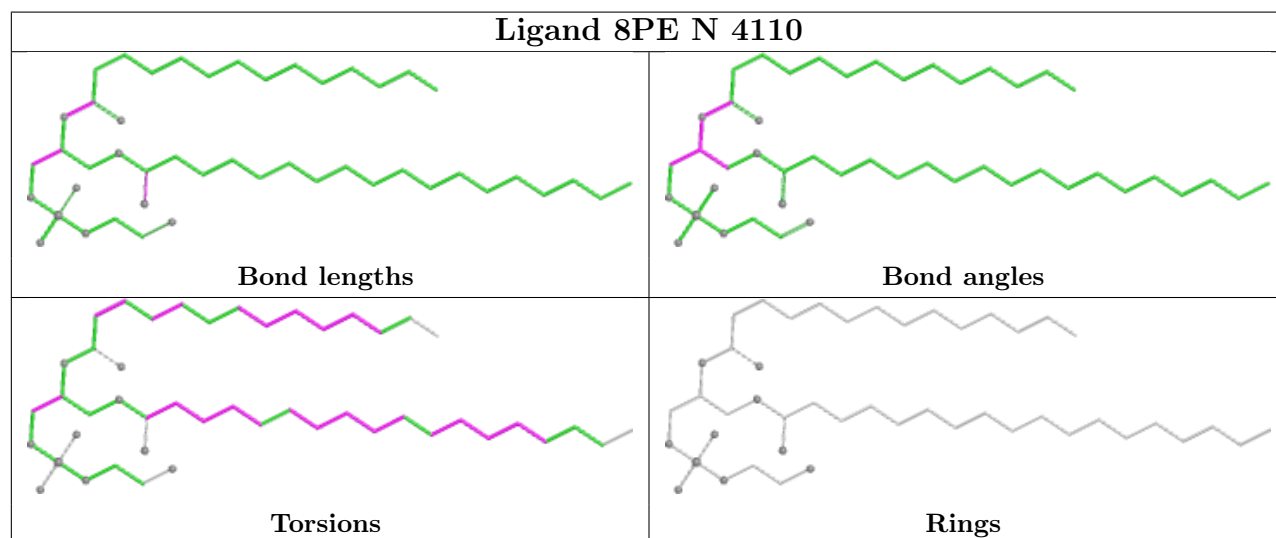
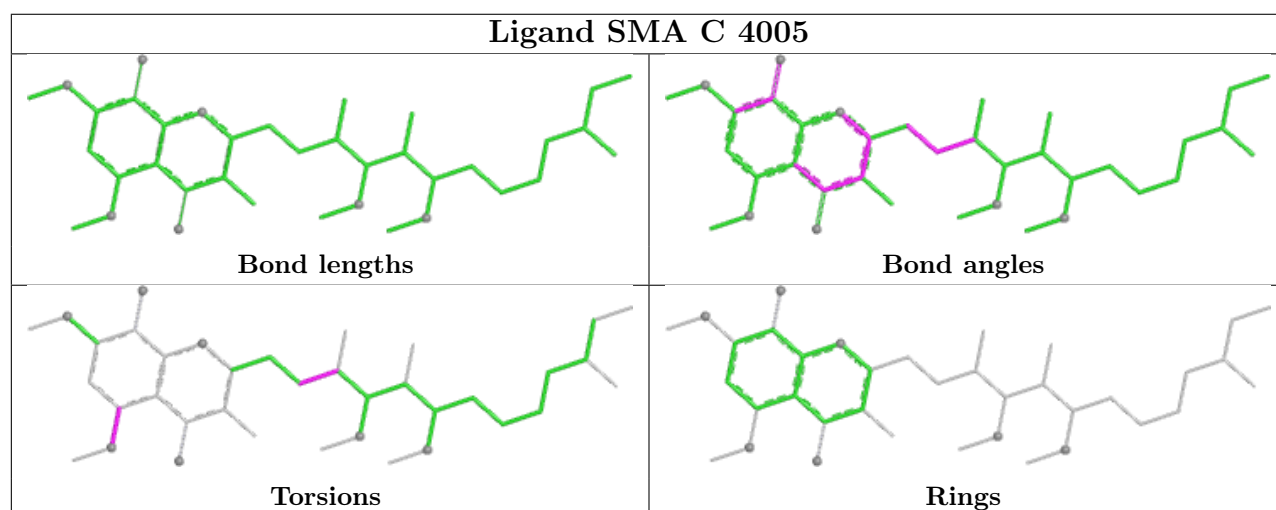
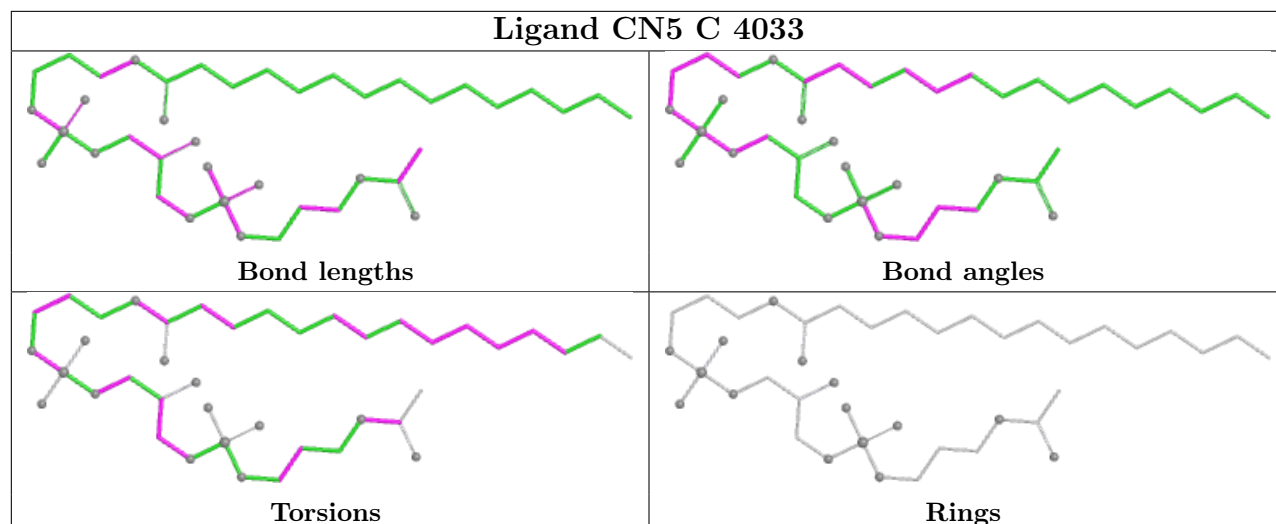


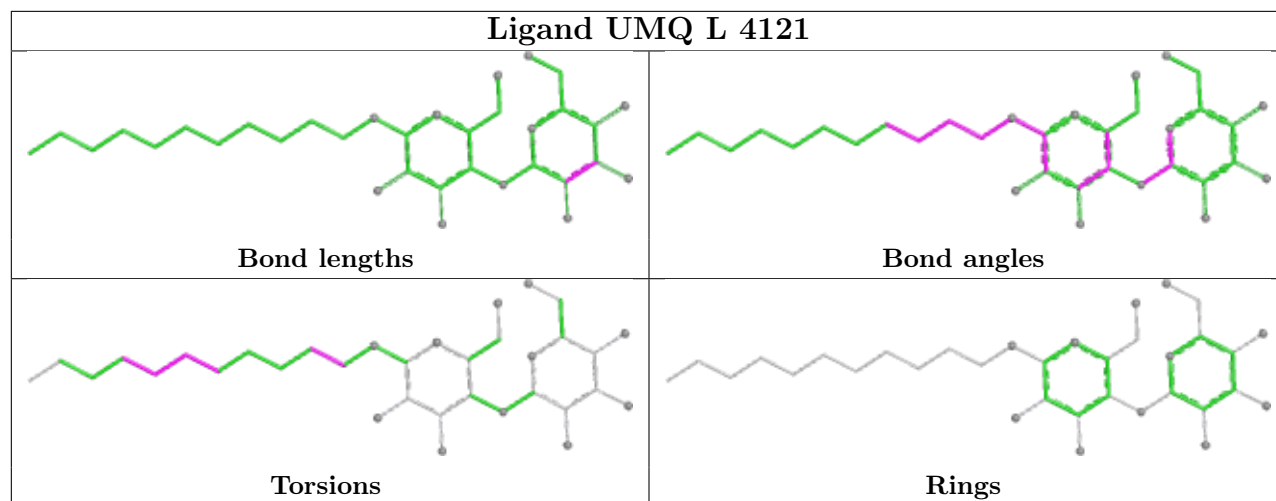
Ligand HEM O 4023



Ligand 7PH O 4114







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.28	106 (24%) 2 1	26, 44, 98, 114	0
1	L	431/431 (100%)	1.14	92 (21%) 2 2	25, 42, 90, 113	0
2	B	352/352 (100%)	1.46	90 (25%) 1 1	30, 47, 73, 114	0
2	M	352/352 (100%)	1.46	92 (26%) 1 1	32, 45, 72, 109	0
3	C	385/385 (100%)	0.02	6 (1%) 70 74	18, 27, 38, 91	0
3	N	385/385 (100%)	-0.07	7 (1%) 67 71	19, 26, 37, 88	0
4	D	248/248 (100%)	0.47	17 (6%) 23 24	25, 35, 57, 83	0
4	O	248/248 (100%)	0.38	19 (7%) 19 21	24, 33, 55, 86	0
5	E	185/185 (100%)	0.90	33 (17%) 4 3	24, 40, 69, 94	0
5	P	185/185 (100%)	1.23	51 (27%) 1 1	24, 41, 80, 93	0
6	F	74/146 (50%)	1.45	22 (29%) 1 1	34, 46, 90, 96	0
6	Q	74/146 (50%)	1.27	14 (18%) 3 3	32, 45, 87, 90	0
7	G	126/126 (100%)	0.63	15 (11%) 9 9	26, 37, 60, 78	0
7	R	126/126 (100%)	0.58	17 (13%) 7 7	23, 34, 62, 80	0
8	H	93/93 (100%)	2.24	40 (43%) 0 0	24, 45, 128, 131	0
8	S	93/93 (100%)	1.88	34 (36%) 1 0	22, 43, 113, 119	0
9	I	57/65 (87%)	1.65	14 (24%) 2 1	34, 42, 83, 100	0
9	T	57/65 (87%)	1.65	17 (29%) 1 1	32, 40, 84, 96	0
10	J	127/127 (100%)	1.92	47 (37%) 1 0	40, 57, 71, 80	0
10	U	127/127 (100%)	2.23	66 (51%) 0 0	42, 59, 73, 82	0
11	K	107/107 (100%)	3.41	81 (75%) 0 0	51, 81, 114, 116	0
11	V	107/107 (100%)	3.87	101 (94%) 0 0	60, 92, 120, 122	0
12	W	107/108 (99%)	2.37	67 (62%) 0 0	29, 62, 87, 99	1 (0%)
All	All	4477/4638 (96%)	1.15	1048 (23%) 2 1	18, 41, 90, 131	1 (0%)

All (1048) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	46	PHE	17.5
1	A	230	LEU	15.8
9	I	57	ALA	13.2
1	L	230	LEU	13.1
2	B	336	ILE	12.6
8	S	49	PHE	11.7
3	C	383	VAL	11.1
11	K	11	LEU	11.0
2	B	338	LEU	11.0
1	A	129	ALA	10.0
8	H	45	VAL	9.9
8	H	51	ARG	9.9
2	M	338	LEU	9.7
8	S	46	PHE	9.6
1	A	228	LEU	9.5
9	T	57	ALA	9.5
2	B	332	VAL	9.1
9	T	58	ALA	9.1
11	K	23	CYS	9.1
8	H	49	PHE	8.4
8	H	37	LEU	8.4
11	V	80	PRO	7.9
8	S	52	PHE	7.9
2	M	332	VAL	7.8
11	K	21	ILE	7.7
11	K	15	LEU	7.7
1	A	234	THR	7.6
8	H	94	VAL	7.6
11	V	15	LEU	7.6
2	M	336	ILE	7.5
11	V	2	ILE	7.5
3	N	383	VAL	7.4
1	L	228	LEU	7.3
1	A	232	THR	7.3
8	H	40	ILE	7.3
1	A	30	THR	7.3
11	V	29	ILE	7.2
11	K	106	ILE	7.2
3	C	384	ASN	7.2
11	V	4	LEU	7.1
1	L	233	GLY	7.0
1	L	237	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
5	P	213	ILE	6.8
11	V	102	THR	6.7
11	K	9	VAL	6.7
11	V	75	ILE	6.7
11	V	19	VAL	6.6
8	S	41	PHE	6.6
11	V	20	THR	6.6
8	S	45	VAL	6.5
1	L	232	THR	6.5
3	N	384	ASN	6.4
8	H	44	ALA	6.3
8	H	52	PHE	6.3
2	B	211	ALA	6.3
11	V	69	THR	6.3
2	M	328	GLN	6.3
11	V	23	CYS	6.2
11	V	7	THR	6.2
11	V	11	LEU	6.1
9	I	56	ILE	6.1
1	L	236	PRO	6.1
10	U	32	GLY	6.1
8	H	47	ASN	6.0
11	K	75	ILE	6.0
1	L	234	THR	5.9
11	K	80	PRO	5.9
1	A	124	PHE	5.9
4	D	286	TRP	5.9
11	K	4	LEU	5.9
8	H	41	PHE	5.9
5	P	49	ALA	5.8
9	I	58	ALA	5.8
2	M	329	ASN	5.8
1	A	237	VAL	5.8
11	V	9	VAL	5.8
1	L	231	GLN	5.8
7	R	127	LYS	5.7
11	K	104	LEU	5.7
1	A	125	ILE	5.7
5	P	92	ALA	5.7
8	H	4	PRO	5.7
1	L	35	GLY	5.7
11	V	78	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
11	K	79	GLU	5.7
2	M	211	ALA	5.7
11	V	66	GLY	5.6
11	V	83	ILE	5.6
6	F	117	LEU	5.6
10	U	68	LEU	5.6
11	K	10	SER	5.6
2	B	339	ASN	5.5
1	A	128	LYS	5.5
8	S	94	VAL	5.5
11	V	92	ILE	5.5
1	A	233	GLY	5.5
11	K	73	LEU	5.5
11	V	106	ILE	5.5
1	L	225	SER	5.5
9	I	2	SER	5.5
1	A	229	SER	5.5
2	B	337	GLU	5.5
1	A	35	GLY	5.4
2	B	334	SER	5.4
2	M	267	LEU	5.4
1	A	37	VAL	5.4
2	M	330	GLU	5.4
11	K	83	ILE	5.4
2	M	335	PRO	5.4
6	Q	117	LEU	5.4
1	A	36	ILE	5.4
8	S	40	ILE	5.4
12	W	1	THR	5.3
2	B	335	PRO	5.3
1	A	27	ALA	5.2
11	K	16	GLY	5.2
11	V	63	SER	5.2
2	M	337	GLU	5.2
5	P	145	ASP	5.2
8	S	44	ALA	5.2
11	K	13	ALA	5.2
11	K	14	SER	5.2
2	M	318	ILE	5.1
5	E	49	ALA	5.1
1	A	29	VAL	5.1
8	H	38	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
12	W	56	ALA	5.1
11	K	94	PHE	5.1
11	K	74	THR	5.1
1	A	214	ILE	5.0
10	U	31	SER	5.0
7	G	127	LYS	5.0
8	H	42	HIS	5.0
2	M	327	VAL	5.0
1	L	380	SER	5.0
1	A	32	LEU	5.0
1	L	32	LEU	5.0
11	V	14	SER	5.0
8	S	37	LEU	5.0
1	A	33	SER	5.0
1	A	381	GLY	5.0
11	K	12	ALA	4.9
10	J	64	LEU	4.9
1	A	236	PRO	4.9
2	B	340	PHE	4.9
1	L	30	THR	4.9
1	L	130	ASN	4.9
11	V	68	GLY	4.9
11	V	5	THR	4.9
8	S	2	GLY	4.9
1	L	129	ALA	4.9
1	L	31	GLN	4.9
11	K	102	THR	4.9
5	P	100	ALA	4.9
11	V	12	ALA	4.9
1	L	76	ILE	4.8
11	V	44	ILE	4.8
8	S	47	ASN	4.8
9	T	56	ILE	4.8
11	K	29	ILE	4.8
11	V	33	LEU	4.8
3	C	385	LYS	4.8
1	A	127	GLN	4.8
2	B	21	ALA	4.8
2	B	154	GLY	4.8
9	T	3	PHE	4.7
11	V	76	SER	4.7
8	S	5	SER	4.7

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Mol	Chain	Res	Type	RSRZ
9	T	2	SER	4.7
4	O	210	PRO	4.7
5	P	211	LYS	4.7
8	H	50	ARG	4.7
1	A	223	ILE	4.7
11	K	2	ILE	4.7
2	M	339	ASN	4.6
12	W	107	CYS	4.6
8	S	42	HIS	4.6
1	L	128	LYS	4.6
6	F	107	ILE	4.6
8	S	39	GLY	4.6
1	A	271	ASN	4.6
1	L	227	ASN	4.6
2	M	331	SER	4.5
11	V	32	PHE	4.5
11	V	18	ARG	4.5
5	P	212	VAL	4.5
1	A	238	LEU	4.5
10	U	30	THR	4.5
1	A	225	SER	4.5
10	J	45	LYS	4.5
11	K	42	GLY	4.5
11	V	13	ALA	4.5
10	U	100	GLU	4.5
1	L	125	ILE	4.5
2	M	250	LEU	4.5
2	B	246	ASN	4.5
1	L	381	GLY	4.5
8	S	48	SER	4.5
11	K	7	THR	4.5
1	A	231	GLN	4.4
8	H	67	TRP	4.4
11	K	40	PRO	4.4
2	M	20	SER	4.4
11	K	100	ALA	4.4
1	A	130	ASN	4.4
11	V	104	LEU	4.4
2	B	318	ILE	4.4
11	V	88	CYS	4.4
5	P	93	LYS	4.4
5	P	90	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
9	I	3	PHE	4.4
1	A	120	LEU	4.4
5	E	103	LEU	4.4
6	Q	107	ILE	4.4
11	V	8	PRO	4.4
11	V	21	ILE	4.4
11	V	31	ASN	4.4
1	L	126	GLN	4.3
8	H	48	SER	4.3
12	W	3	PHE	4.3
5	P	208	ASP	4.3
10	J	52	ILE	4.3
10	U	44	ASN	4.3
1	A	226	LYS	4.3
6	F	75	THR	4.3
1	L	239	LYS	4.3
6	F	119	HIS	4.3
5	P	43	LEU	4.3
10	J	68	LEU	4.3
2	M	343	VAL	4.3
11	K	69	THR	4.3
9	T	54	ALA	4.3
5	P	123	PRO	4.3
1	L	120	LEU	4.2
4	O	286	TRP	4.2
11	K	77	ASN	4.2
1	A	76	ILE	4.2
3	C	223	SER	4.2
6	F	115	ALA	4.2
8	H	39	GLY	4.2
12	W	34	GLY	4.2
5	P	98	LEU	4.2
1	A	34	ASN	4.1
1	L	27	ALA	4.1
9	I	9	THR	4.1
11	K	20	THR	4.1
11	V	97	THR	4.1
11	K	17	ASP	4.1
7	G	24	LEU	4.1
5	P	152	TRP	4.1
9	T	26	PHE	4.1
2	B	343	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
11	V	84	ALA	4.1
1	A	31	GLN	4.1
2	B	17	LEU	4.1
11	V	79	GLU	4.1
2	M	340	PHE	4.1
1	L	36	ILE	4.1
4	D	212	SER	4.1
4	O	309	LYS	4.1
11	V	39	LYS	4.1
1	L	271	ASN	4.1
5	P	103	LEU	4.1
11	V	47	LEU	4.1
10	J	86	VAL	4.0
11	V	53	ARG	4.0
8	S	4	PRO	4.0
1	L	222	SER	4.0
2	M	141	SER	4.0
2	M	249	SER	4.0
5	P	97	ASN	4.0
12	W	2	GLU	4.0
1	A	219	LEU	4.0
1	L	238	LEU	4.0
5	E	210	ASP	4.0
5	E	213	ILE	4.0
5	P	207	PHE	4.0
5	P	44	LYS	4.0
1	L	226	LYS	4.0
7	R	20	VAL	4.0
9	I	54	ALA	4.0
11	V	51	THR	4.0
11	V	6	GLN	4.0
5	E	44	LYS	4.0
2	M	333	SER	4.0
11	K	72	SER	4.0
1	L	29	VAL	4.0
10	J	30	THR	3.9
11	V	64	GLY	3.9
11	K	70	ASP	3.9
5	E	47	ASN	3.9
1	L	33	SER	3.9
11	K	25	ALA	3.9
10	J	41	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	117	LEU	3.9
11	K	78	LEU	3.9
11	V	54	LEU	3.9
1	A	215	LYS	3.9
8	S	86	ARG	3.9
2	M	246	ASN	3.9
1	A	235	LYS	3.9
10	J	104	VAL	3.9
12	W	55	ASP	3.9
11	V	30	ASN	3.8
4	D	208	LEU	3.8
11	V	96	TRP	3.8
1	A	270	VAL	3.8
5	P	94	VAL	3.8
11	K	19	VAL	3.8
1	L	122	GLN	3.8
12	W	21[A]	GLN	3.8
2	B	267	LEU	3.8
7	R	2	PRO	3.8
11	K	68	GLY	3.8
5	P	91	MET	3.8
1	L	127	GLN	3.8
2	M	266	GLU	3.8
11	K	22	SER	3.8
11	V	65	SER	3.8
6	Q	119	HIS	3.8
2	B	155	LEU	3.8
4	O	141	GLN	3.8
2	B	342	ALA	3.8
4	O	137	GLU	3.8
1	L	457	TRP	3.8
5	P	101	ILE	3.8
6	F	106	LYS	3.8
12	W	7	SER	3.8
1	A	131	LEU	3.7
10	U	64	LEU	3.7
11	V	73	LEU	3.7
12	W	106	ALA	3.7
11	V	35	TRP	3.7
12	W	76	PRO	3.7
11	K	5	THR	3.7
11	K	71	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
8	S	50	ARG	3.7
12	W	22	CYS	3.7
2	B	366	ASP	3.7
6	F	144	ASP	3.7
2	B	327	VAL	3.7
2	B	212	GLY	3.7
2	B	347	LYS	3.7
12	W	92	LYS	3.7
5	E	89	LEU	3.7
11	K	84	ALA	3.7
10	J	63	SER	3.7
11	V	70	ASP	3.7
1	L	90	GLY	3.7
8	H	2	GLY	3.7
10	U	43	GLY	3.7
11	K	32	PHE	3.7
11	K	76	SER	3.6
11	V	100	ALA	3.6
12	W	8	ALA	3.6
10	U	55	VAL	3.6
1	L	124	PHE	3.6
1	A	79	SER	3.6
2	M	31	LEU	3.6
3	N	385	LYS	3.6
2	B	330	GLU	3.6
12	W	83	THR	3.6
11	K	54	LEU	3.6
12	W	42	GLY	3.6
11	V	3	GLU	3.6
11	K	85	THR	3.6
1	A	118	ASP	3.6
11	K	107	LYS	3.6
12	W	9	LYS	3.6
10	U	123	ALA	3.5
11	V	25	ALA	3.5
1	L	229	SER	3.5
5	E	48	ASP	3.5
10	U	85	SER	3.5
10	U	87	THR	3.5
11	K	43	THR	3.5
11	V	74	THR	3.5
10	U	120	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	L	235	LYS	3.5
11	V	1	ASP	3.5
10	U	63	SER	3.5
10	U	103	SER	3.5
11	V	22	SER	3.5
1	L	115	LYS	3.5
10	J	87	THR	3.5
11	V	107	LYS	3.5
1	L	214	ILE	3.5
10	U	29	ILE	3.5
11	K	44	ILE	3.5
1	L	34	ASN	3.5
7	G	21	LEU	3.5
4	O	308	ARG	3.5
2	M	217	SER	3.5
3	N	223	SER	3.5
8	S	54	SER	3.5
10	U	45	LYS	3.5
11	K	65	SER	3.5
10	J	100	GLU	3.5
2	B	193	VAL	3.5
2	M	17	LEU	3.5
7	R	21	LEU	3.5
8	S	51	ARG	3.5
1	L	135	SER	3.4
8	S	43	ASN	3.4
10	U	70	ILE	3.4
7	R	16	LEU	3.4
12	W	14	LEU	3.4
10	J	75	SER	3.4
1	A	172	THR	3.4
10	U	42	PRO	3.4
8	H	86	ARG	3.4
1	A	220	VAL	3.4
2	B	359	VAL	3.4
7	G	26	VAL	3.4
8	H	92	VAL	3.4
11	V	98	PHE	3.4
2	B	217	SER	3.4
2	B	333	SER	3.4
2	B	368	LEU	3.4
1	A	227	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
7	G	90	ARG	3.4
9	T	55	ARG	3.4
1	A	224	GLU	3.4
2	B	266	GLU	3.4
2	M	345	ASP	3.4
11	V	101	GLY	3.4
7	G	20	VAL	3.4
10	U	104	VAL	3.4
2	M	342	ALA	3.4
1	A	221	ASN	3.4
10	U	127	PRO	3.4
12	W	13	THR	3.4
11	V	91	HIS	3.3
11	K	81	GLU	3.3
2	M	292	GLN	3.3
5	P	209	GLY	3.3
11	K	66	GLY	3.3
1	L	84	ALA	3.3
8	S	67	TRP	3.3
2	M	150	THR	3.3
5	P	122	THR	3.3
1	A	212	GLY	3.3
10	J	85	SER	3.3
11	V	86	TYR	3.3
10	U	52	ILE	3.3
2	M	310	LYS	3.3
11	V	94	PHE	3.3
10	J	122	SER	3.3
11	V	50	TYR	3.3
5	E	51	LYS	3.3
11	K	1	ASP	3.3
2	B	22	ARG	3.3
11	K	18	ARG	3.3
2	M	189	GLY	3.3
12	W	11	GLY	3.3
2	B	320	TYR	3.2
10	U	101	TYR	3.2
2	M	366	ASP	3.2
1	A	134	SER	3.2
8	S	38	GLN	3.2
1	A	150	ASP	3.2
6	Q	115	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
12	W	86	ALA	3.2
2	B	261	THR	3.2
8	S	3	PRO	3.2
11	V	40	PRO	3.2
11	V	77	ASN	3.2
1	A	380	SER	3.2
1	A	122	GLN	3.2
2	M	22	ARG	3.2
5	P	45	GLU	3.2
11	V	85	THR	3.2
2	B	221	PRO	3.2
2	M	216	VAL	3.2
2	B	189	GLY	3.2
2	M	188	SER	3.2
12	W	6	GLY	3.2
11	V	62	PHE	3.2
11	V	24	ARG	3.2
1	A	115	LYS	3.1
2	M	321	THR	3.1
11	V	103	LYS	3.1
1	A	44	PRO	3.1
11	V	71	TYR	3.1
5	P	214	VAL	3.1
10	U	28	SER	3.1
6	F	113	GLY	3.1
11	K	87	PHE	3.1
2	B	345	ASP	3.1
1	A	28	GLU	3.1
2	M	344	LYS	3.1
2	B	329	ASN	3.1
5	E	46	ASN	3.1
5	P	47	ASN	3.1
2	M	261	THR	3.1
1	A	39	ALA	3.1
10	U	92	ALA	3.1
4	D	210	PRO	3.1
2	M	74	LEU	3.1
9	T	12	LYS	3.1
11	V	38	GLN	3.1
5	P	46	ASN	3.1
2	M	214	SER	3.1
2	M	315	SER	3.1

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Mol	Chain	Res	Type	RSRZ
4	O	307	PRO	3.1
2	B	271	ILE	3.1
1	L	270	VAL	3.1
2	M	19	VAL	3.1
5	P	111	TRP	3.1
11	K	47	LEU	3.1
12	W	73	LEU	3.1
11	K	6	GLN	3.1
12	W	87	PHE	3.1
2	B	331	SER	3.1
11	K	26	SER	3.1
5	E	90	ALA	3.1
5	P	204	ALA	3.1
1	A	218	ASP	3.0
4	O	208	LEU	3.0
2	B	19	VAL	3.0
7	R	125	VAL	3.0
1	L	221	ASN	3.0
8	H	56	PHE	3.0
1	L	224	GLU	3.0
2	B	190	GLU	3.0
7	R	126	SER	3.0
11	V	72	SER	3.0
10	J	93	THR	3.0
10	U	88	THR	3.0
11	K	51	THR	3.0
5	E	43	LEU	3.0
6	F	74	VAL	3.0
8	H	90	GLU	3.0
11	K	96	TRP	3.0
1	L	123	SER	3.0
9	T	5	SER	3.0
11	V	87	PHE	3.0
12	W	54	THR	3.0
12	W	35	PRO	3.0
1	A	126	GLN	3.0
6	Q	106	LYS	3.0
11	K	39	LYS	3.0
5	E	100	ALA	3.0
10	U	59	ASN	3.0
1	A	401	LEU	3.0
4	O	123	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
11	K	33	LEU	3.0
8	H	68	TYR	3.0
11	V	49	TYR	3.0
2	M	79	LYS	3.0
4	D	211	GLY	3.0
11	K	101	GLY	3.0
12	W	29	GLY	3.0
10	J	42	PRO	3.0
2	M	166	ARG	3.0
11	V	81	GLU	3.0
10	U	40	LEU	2.9
10	U	81	LEU	2.9
5	P	147	VAL	2.9
11	V	10	SER	2.9
12	W	53	TYR	2.9
5	P	105	LYS	2.9
6	F	116	ASP	2.9
10	J	43	GLY	2.9
10	J	123	ALA	2.9
12	W	5	ALA	2.9
10	J	38	ILE	2.9
1	L	131	LEU	2.9
11	V	93	LYS	2.9
1	L	218	ASP	2.9
10	J	125	ARG	2.9
10	U	66	ASP	2.9
2	M	179	VAL	2.9
8	S	92	VAL	2.9
6	F	114	TYR	2.9
10	U	33	TYR	2.9
12	W	51	TYR	2.9
2	B	150	THR	2.9
10	U	74	THR	2.9
1	A	213	ASN	2.9
4	D	308	ARG	2.9
2	M	149	ILE	2.9
5	P	48	ASP	2.9
10	U	38	ILE	2.9
12	W	93	GLU	2.9
1	L	394	VAL	2.9
2	B	305	VAL	2.9
5	E	88	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	92	ALA	2.9
1	L	240	LYS	2.9
2	M	202	ASP	2.9
2	M	334	SER	2.9
12	W	108	GLU	2.9
10	J	83	LEU	2.9
1	L	220	VAL	2.8
10	J	12	VAL	2.8
5	P	205	TYR	2.8
8	H	3	PRO	2.8
2	M	128	ARG	2.8
11	K	98	PHE	2.8
4	O	235	GLU	2.8
1	A	135	SER	2.8
1	A	403	LEU	2.8
10	U	83	LEU	2.8
12	W	90	LEU	2.8
5	P	104	GLY	2.8
10	U	10	GLY	2.8
10	U	106	GLY	2.8
1	A	38	VAL	2.8
2	M	86	TYR	2.8
2	B	326	ALA	2.8
8	H	54	SER	2.8
10	U	41	PHE	2.8
10	U	69	SER	2.8
11	V	99	GLY	2.8
1	L	202	LEU	2.8
12	W	58	ILE	2.8
12	W	81	PRO	2.8
2	B	255	VAL	2.8
12	W	33	VAL	2.8
1	A	153	ASP	2.8
1	L	153	ASP	2.8
1	L	134	SER	2.8
10	J	121	SER	2.8
10	U	53	SER	2.8
11	K	27	GLN	2.8
1	L	398	GLY	2.8
2	M	212	GLY	2.8
10	J	3	LYS	2.8
1	A	186	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	395	LEU	2.8
2	B	280	THR	2.8
6	F	112	PRO	2.8
10	J	24	VAL	2.8
10	U	118	VAL	2.8
4	D	309	LYS	2.7
10	U	65	LYS	2.7
12	W	78	LYS	2.7
5	E	45	GLU	2.7
6	Q	97	HIS	2.7
8	H	78	GLU	2.7
10	J	106	GLY	2.7
2	B	308	LEU	2.7
1	L	114	ASP	2.7
1	L	44	PRO	2.7
1	A	195	SER	2.7
7	R	22	SER	2.7
1	L	208	VAL	2.7
11	K	31	ASN	2.7
10	J	65	LYS	2.7
2	M	282	GLY	2.7
11	V	16	GLY	2.7
1	A	72	LEU	2.7
8	H	60	LEU	2.7
11	K	92	ILE	2.7
10	U	15	SER	2.7
4	O	140	GLU	2.7
12	W	10	LYS	2.7
12	W	84	LYS	2.7
1	L	37	VAL	2.7
2	B	245	VAL	2.7
11	K	97	THR	2.7
1	A	395	LEU	2.7
7	R	18	SER	2.7
2	B	79	LYS	2.7
11	V	45	LYS	2.7
2	M	193	VAL	2.7
2	M	245	VAL	2.7
6	F	105	VAL	2.7
11	V	36	TYR	2.6
2	B	346	PHE	2.6
9	T	9	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	183	GLU	2.6
6	Q	100	GLU	2.6
2	B	214	SER	2.6
11	K	63	SER	2.6
12	W	94	LYS	2.6
2	B	250	LEU	2.6
9	I	6	LEU	2.6
11	V	46	LEU	2.6
1	A	216	HIS	2.6
11	K	91	HIS	2.6
1	L	144	VAL	2.6
5	P	96	VAL	2.6
6	Q	113	GLY	2.6
11	K	99	GLY	2.6
1	A	114	ASP	2.6
1	L	150	ASP	2.6
11	V	28	ASP	2.6
11	V	61	ARG	2.6
10	U	89	GLU	2.6
7	G	17	LYS	2.6
10	U	91	THR	2.6
12	W	104	LYS	2.6
10	J	59	ASN	2.6
10	U	62	PRO	2.6
11	K	8	PRO	2.6
11	V	90	HIS	2.6
1	A	91	LEU	2.6
9	T	6	LEU	2.6
2	B	311	GLY	2.6
11	V	17	ASP	2.6
6	F	79	GLU	2.6
2	M	21	ALA	2.6
11	K	58	VAL	2.6
2	B	299	SER	2.6
8	H	43	ASN	2.6
10	U	60	TYR	2.6
10	J	127	PRO	2.6
12	W	41	PHE	2.6
1	A	457	TRP	2.6
10	U	124	TRP	2.6
2	B	365	LEU	2.6
2	M	215	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
8	H	91	ARG	2.6
12	W	99	LEU	2.6
1	L	118	ASP	2.6
1	L	217	GLU	2.6
2	M	135	GLU	2.6
7	R	23	LYS	2.6
5	P	42	VAL	2.6
4	O	212	SER	2.6
10	U	121	SER	2.6
11	V	26	SER	2.6
1	A	113	THR	2.6
2	B	18	THR	2.6
4	O	185	HIS	2.5
9	I	26	PHE	2.5
11	V	105	GLU	2.5
3	N	160	ASP	2.5
10	J	124	TRP	2.5
11	K	35	TRP	2.5
10	U	3	LYS	2.5
12	W	28	GLY	2.5
2	M	248	ALA	2.5
9	T	4	SER	2.5
1	A	42	HIS	2.5
6	F	97	HIS	2.5
11	V	58	VAL	2.5
4	D	244	THR	2.5
10	J	74	THR	2.5
4	O	126	ARG	2.5
2	B	328	GLN	2.5
5	E	112	GLN	2.5
4	D	307	PRO	2.5
7	G	2	PRO	2.5
11	K	88	CYS	2.5
2	B	129	TYR	2.5
5	P	41	ASP	2.5
10	U	102	TYR	2.5
11	V	82	ASP	2.5
12	W	4	LYS	2.5
7	G	16	LEU	2.5
5	E	104	GLY	2.5
11	V	48	ILE	2.5
12	W	80	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	203	ASN	2.5
1	L	42	HIS	2.5
12	W	38	HIS	2.5
2	M	263	ALA	2.5
2	B	133	VAL	2.5
2	B	216	VAL	2.5
2	M	26	THR	2.5
6	F	147	LYS	2.5
2	B	86	TYR	2.5
2	B	264	LEU	2.5
2	B	323	LEU	2.5
2	M	205	LEU	2.5
3	N	169	PHE	2.5
5	P	215	GLY	2.5
2	M	251	ALA	2.5
2	M	164	VAL	2.5
2	B	218	LYS	2.5
2	M	313	ASP	2.5
11	V	34	ASN	2.4
1	L	117	LEU	2.4
7	R	24	LEU	2.4
1	A	133	SER	2.4
7	R	123	ILE	2.4
8	H	7	LYS	2.4
8	S	7	LYS	2.4
11	K	93	LYS	2.4
11	V	56	ALA	2.4
12	W	48	ALA	2.4
1	A	394	VAL	2.4
2	M	255	VAL	2.4
3	C	157	VAL	2.4
4	D	138	PRO	2.4
5	E	42	VAL	2.4
11	V	95	PRO	2.4
1	L	404	GLY	2.4
5	P	206	GLU	2.4
6	F	110	GLN	2.4
1	A	123	SER	2.4
10	U	99	SER	2.4
8	H	53	LYS	2.4
12	W	16	LYS	2.4
11	K	48	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	M	195	ALA	2.4
6	Q	112	PRO	2.4
8	H	36	PRO	2.4
1	L	209	VAL	2.4
2	M	220	GLU	2.4
7	R	97	GLN	2.4
8	S	15	HIS	2.4
12	W	23	HIS	2.4
1	L	399	SER	2.4
2	B	315	SER	2.4
11	V	52	SER	2.4
1	L	215	LYS	2.4
2	M	347	LYS	2.4
7	G	14	TYR	2.4
2	M	23	ASP	2.4
2	B	166	ARG	2.4
2	M	28	ILE	2.4
1	L	49	ALA	2.4
6	F	99	GLU	2.4
8	H	55	GLN	2.4
2	M	359	VAL	2.4
6	F	95	VAL	2.4
11	K	64	GLY	2.4
1	A	94	SER	2.4
1	A	222	SER	2.4
1	A	80	LYS	2.4
1	A	240	LYS	2.4
1	L	400	LYS	2.4
11	K	103	LYS	2.4
5	E	40	ASP	2.3
6	F	80	ASP	2.3
10	J	46	LEU	2.3
1	L	101	PHE	2.3
2	M	351	PHE	2.3
3	C	307	PHE	2.3
5	E	122	THR	2.3
12	W	74	THR	2.3
12	W	12	ALA	2.3
5	E	97	ASN	2.3
10	J	56	GLY	2.3
2	B	213	LYS	2.3
5	P	110	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
9	I	50	LYS	2.3
2	B	102	VAL	2.3
1	A	109	LEU	2.3
1	L	219	LEU	2.3
12	W	24	THR	2.3
5	E	207	PHE	2.3
5	E	204	ALA	2.3
11	K	56	ALA	2.3
5	E	101	ILE	2.3
10	J	29	ILE	2.3
11	V	59	PRO	2.3
12	W	30	PRO	2.3
12	W	89	GLY	2.3
2	B	128	ARG	2.3
10	U	67	ARG	2.3
1	A	405	GLU	2.3
12	W	103	LEU	2.3
1	L	113	THR	2.3
2	B	120	THR	2.3
10	J	116	THR	2.3
6	Q	114	TYR	2.3
10	J	102	TYR	2.3
2	B	263	ALA	2.3
2	M	311	GLY	2.3
7	G	10	ARG	2.3
10	U	75	SER	2.3
11	V	60	SER	2.3
6	Q	118	GLU	2.3
5	E	94	VAL	2.3
9	T	52	VAL	2.3
10	U	12	VAL	2.3
2	M	137	CYS	2.3
1	L	397	LYS	2.3
11	K	24	ARG	2.2
1	A	173	PRO	2.2
2	B	135	GLU	2.2
2	M	24	ALA	2.2
5	P	102	PRO	2.2
2	M	273	SER	2.2
1	L	223	ILE	2.2
2	M	271	ILE	2.2
7	R	118	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
9	I	29	GLN	2.2
2	B	179	VAL	2.2
2	B	201	VAL	2.2
6	Q	74	VAL	2.2
6	Q	95	VAL	2.2
7	G	125	VAL	2.2
4	O	67	HIS	2.2
1	A	296	ARG	2.2
10	J	22	CYS	2.2
8	H	87	GLU	2.2
10	U	11	LEU	2.2
1	L	94	SER	2.2
1	L	133	SER	2.2
4	D	160	PRO	2.2
8	S	6	GLY	2.2
1	A	206	ALA	2.2
2	B	251	ALA	2.2
5	E	41	ASP	2.2
2	M	78	PHE	2.2
10	U	107	TYR	2.2
10	J	70	ILE	2.2
2	B	310	LYS	2.2
2	B	344	LYS	2.2
2	M	222	LYS	2.2
2	M	312	LYS	2.2
8	H	35	LYS	2.2
2	B	232	ARG	2.2
2	M	199	ARG	2.2
1	A	144	VAL	2.2
1	A	384	VAL	2.2
2	M	190	GLU	2.2
6	F	118	GLU	2.2
2	B	112	THR	2.2
10	U	96	CYS	2.2
1	L	91	LEU	2.2
10	U	46	LEU	2.2
1	A	112	SER	2.2
1	L	45	SER	2.2
12	W	88	GLY	2.2
2	M	129	TYR	2.2
5	P	202	ILE	2.2
2	M	218	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
5	P	120	HIS	2.2
9	T	50	LYS	2.2
10	U	54	ASN	2.2
1	A	217	GLU	2.2
2	B	196	ASP	2.2
1	A	108	SER	2.2
9	I	5	SER	2.2
1	A	202	LEU	2.2
8	H	57	LEU	2.2
12	W	46	GLY	2.2
1	A	242	ALA	2.2
5	P	136	ALA	2.2
10	J	108	ALA	2.2
2	B	153	LYS	2.2
9	I	55	ARG	2.2
9	T	13	ARG	2.2
10	J	76	LYS	2.2
5	P	124	HIS	2.1
2	B	325	ASN	2.1
10	U	95	TYR	2.1
2	B	304	ILE	2.1
11	V	37	GLN	2.1
2	M	341	ASP	2.1
10	J	66	ASP	2.1
2	M	133	VAL	2.1
2	M	187	VAL	2.1
2	M	238	VAL	2.1
10	U	21	THR	2.1
7	G	126	SER	2.1
10	U	122	SER	2.1
2	B	137	CYS	2.1
1	L	424	LYS	2.1
4	O	209	PRO	2.1
8	S	60	LEU	2.1
8	S	75	GLU	2.1
12	W	26	GLU	2.1
1	L	39	ALA	2.1
11	K	30	ASN	2.1
10	U	27	TYR	2.1
10	U	51	TYR	2.1
2	B	26	THR	2.1
5	E	111	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
10	J	15	SER	2.1
1	A	207	VAL	2.1
1	A	208	VAL	2.1
1	A	404	GLY	2.1
2	B	33	VAL	2.1
4	D	239	GLY	2.1
10	U	56	GLY	2.1
12	W	50	GLY	2.1
5	E	93	LYS	2.1
6	Q	79	GLU	2.1
8	H	88	GLU	2.1
8	H	15	HIS	2.1
1	A	145	LEU	2.1
2	B	314	LEU	2.1
6	F	87	ASN	2.1
4	D	207	ALA	2.1
5	P	144	ALA	2.1
7	G	97	GLN	2.1
5	P	210	ASP	2.1
1	L	296	ARG	2.1
12	W	96	ARG	2.1
1	L	89	GLU	2.1
4	D	123	GLU	2.1
4	O	131	GLU	2.1
1	L	43	ASN	2.1
4	D	251	VAL	2.1
5	E	212	VAL	2.1
8	S	72	ASN	2.1
10	U	77	ASN	2.1
4	D	141	GLN	2.1
5	P	115	PRO	2.1
7	R	27	PRO	2.1
8	S	36	PRO	2.1
1	A	49	ALA	2.1
1	A	387	ALA	2.1
5	E	99	ALA	2.1
1	L	79	SER	2.0
2	B	309	LYS	2.0
5	E	138	LYS	2.0
8	S	90	GLU	2.0
9	I	45	LYS	2.0
10	J	89	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
7	R	14	TYR	2.0
12	W	79	TYR	2.0
12	W	85	MET	2.0
4	O	239	GLY	2.0
11	V	42	GLY	2.0
12	W	39	GLY	2.0
12	W	82	GLY	2.0
1	A	121	ASN	2.0
2	M	252	GLN	2.0
9	T	29	GLN	2.0
2	B	47	VAL	2.0
5	P	107	VAL	2.0
1	A	132	LEU	2.0
1	L	193	LEU	2.0
2	M	348	LEU	2.0
5	P	89	LEU	2.0
10	J	40	LEU	2.0
10	J	96	CYS	2.0
5	P	99	ALA	2.0
8	H	84	ALA	2.0
10	J	73	ASP	2.0
12	W	91	LYS	2.0
1	L	195	SER	2.0
7	G	22	SER	2.0
12	W	52	SER	2.0
1	A	137	PHE	2.0
1	A	396	ILE	2.0
1	L	410	ILE	2.0
2	B	223	PHE	2.0
3	N	307	PHE	2.0
1	A	361	THR	2.0
4	O	127	ASN	2.0
5	E	209	GLY	2.0
10	J	10	GLY	2.0
11	V	43	THR	2.0
8	S	68	TYR	2.0
1	A	85	VAL	2.0
2	M	201	VAL	2.0
4	D	126	ARG	2.0
7	R	90	ARG	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.

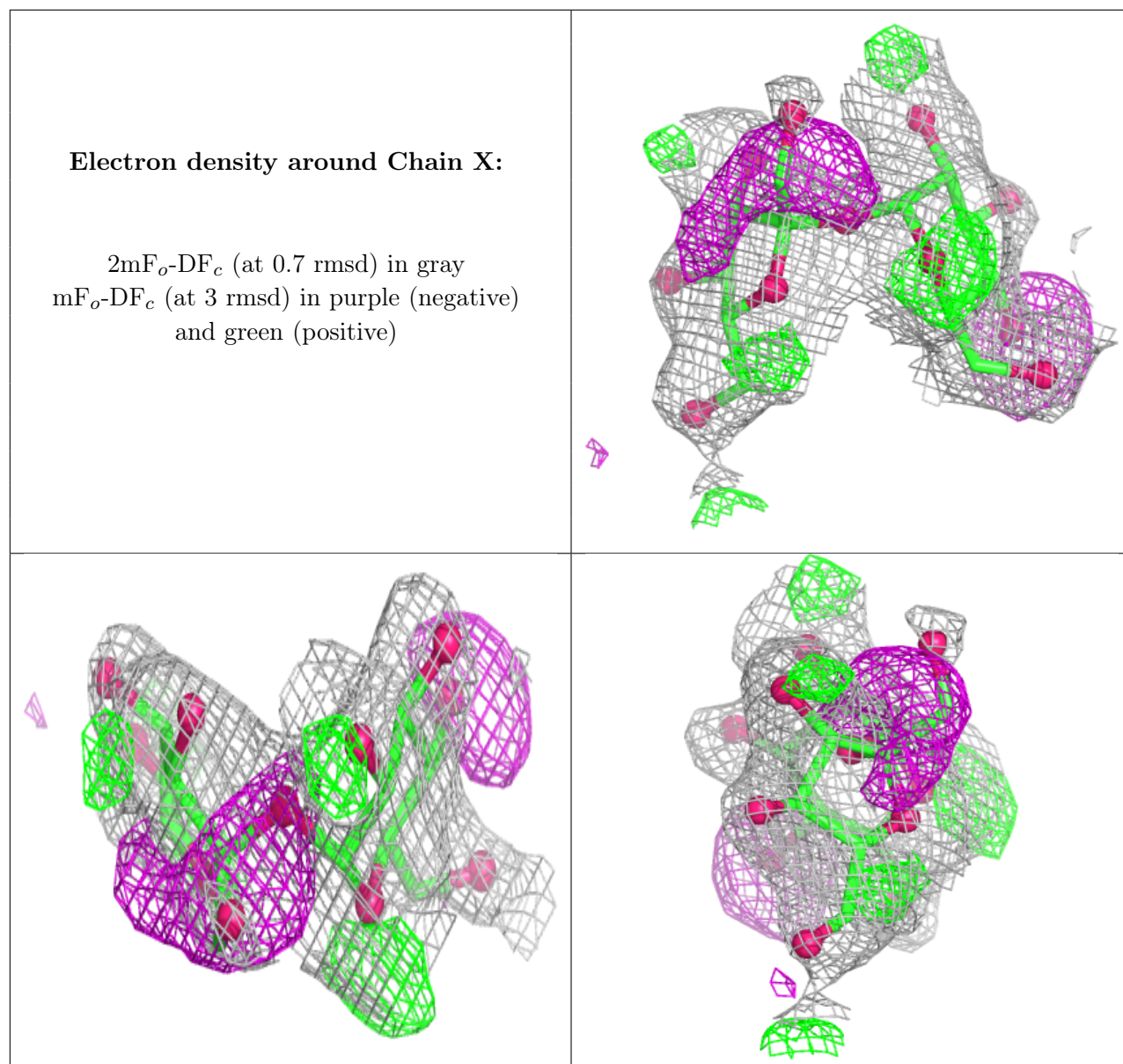
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	M3L	W	77	12/13	0.71	0.22	64,68,72,72	0

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(Å ²)	Q<0.9
13	GLC	X	1	11/12	0.70	0.23	70,71,73,76	0
13	FRU	X	2	12/12	0.76	0.19	68,69,72,72	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(Å ²)	Q<0.9
20	CN5	C	4033	41/41	0.70	0.23	76,79,85,86	0
18	8PE	N	4110	47/47	0.83	0.17	43,51,65,67	0
18	8PE	C	4010	47/47	0.83	0.15	39,50,59,60	0
14	6PH	L	4113	40/40	0.84	0.15	51,55,67,68	0
22	CN3	D	4031	55/55	0.84	0.18	48,62,70,71	0

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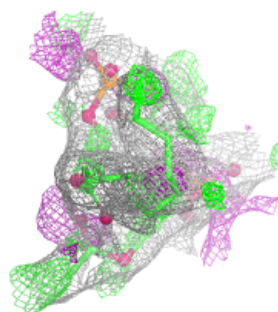
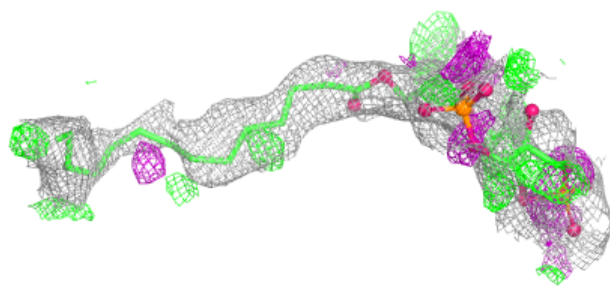
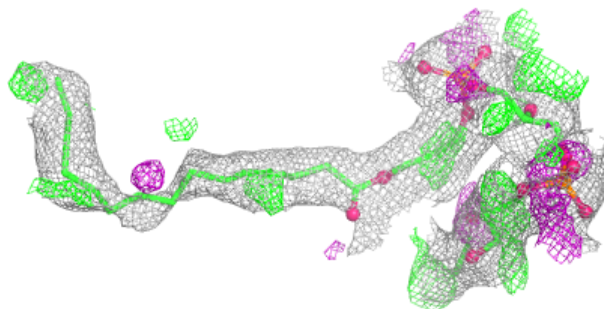
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CN3	N	4131	55/55	0.86	0.17	39,58,66,69	0
19	9PE	N	4111	40/40	0.87	0.14	39,47,62,66	0
14	6PH	A	4013	40/40	0.87	0.14	48,55,61,61	0
19	9PE	C	4011	40/40	0.89	0.13	39,46,70,72	0
21	7PH	O	4114	38/38	0.90	0.11	40,44,52,52	0
16	HEM	W	4026	43/43	0.90	0.15	46,50,54,55	0
21	7PH	D	4014	38/38	0.90	0.12	43,46,62,63	0
15	UMQ	A	4021	34/34	0.92	0.10	32,36,55,56	0
15	UMQ	L	4121	34/34	0.92	0.10	33,35,57,58	0
17	SMA	N	4025	37/37	0.95	0.06	21,24,30,33	0
17	SMA	C	4005	37/37	0.97	0.05	22,24,31,34	0
16	HEM	D	4003	43/43	0.98	0.07	23,29,33,34	0
16	HEM	N	4021	43/43	0.98	0.06	16,20,25,27	0
16	HEM	N	4022	43/43	0.98	0.06	15,18,26,28	0
16	HEM	O	4023	43/43	0.98	0.06	25,28,30,33	0
16	HEM	C	4001	43/43	0.99	0.05	16,21,26,30	0
16	HEM	C	4002	43/43	0.99	0.05	17,20,24,28	0
23	FES	E	4004	4/4	0.99	0.04	27,27,28,31	0
23	FES	P	4024	4/4	0.99	0.04	28,29,31,32	0

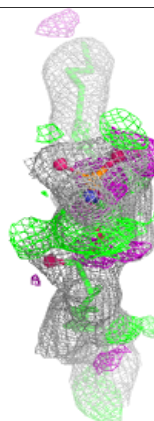
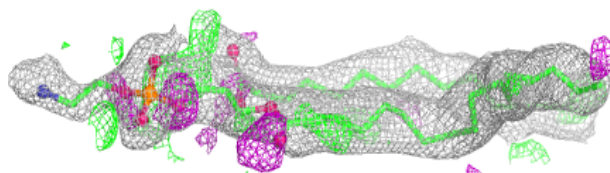
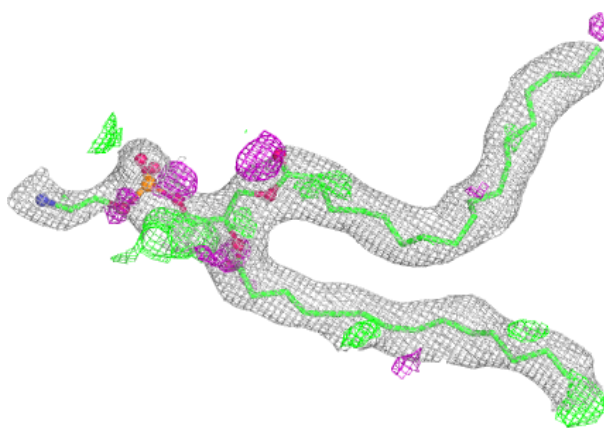
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CN5 C 4033:

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

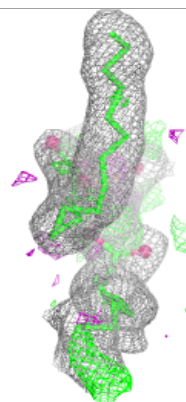
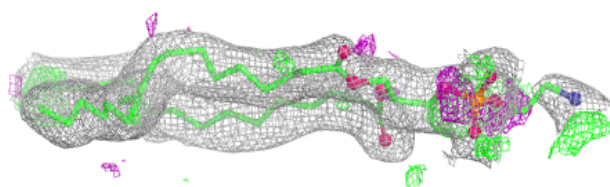
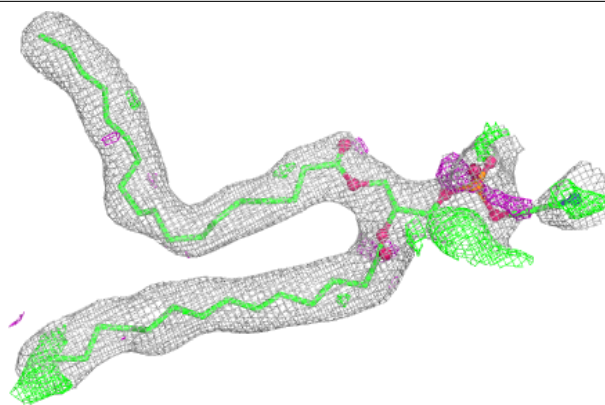
**Electron density around 8PE N 4110:**

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

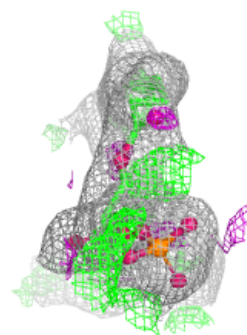
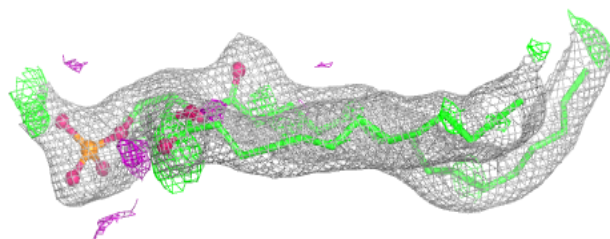
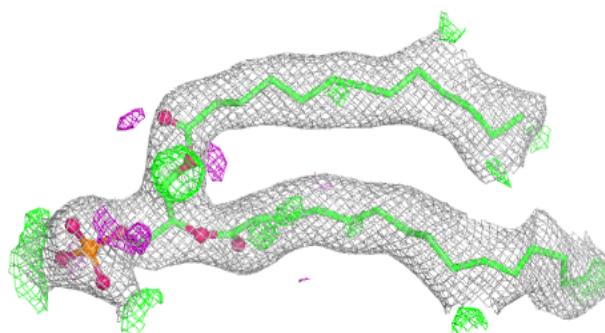


Electron density around 8PE C 4010:

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

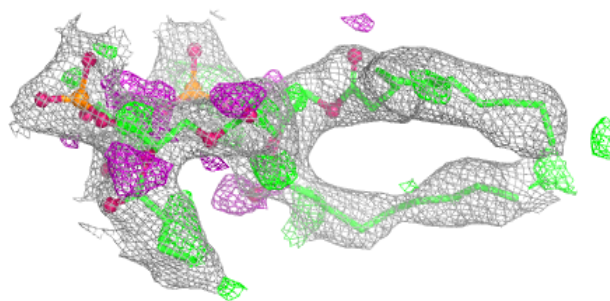
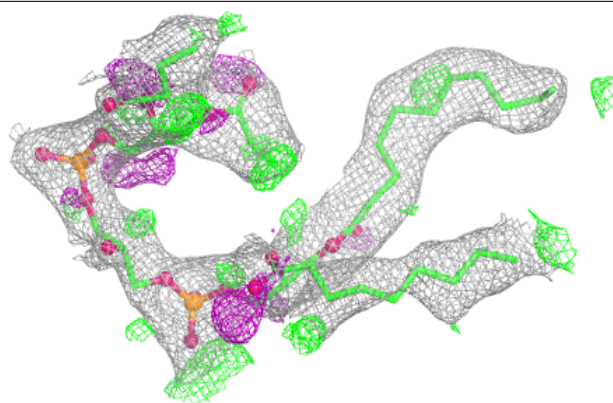
**Electron density around 6PH L 4113:**

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

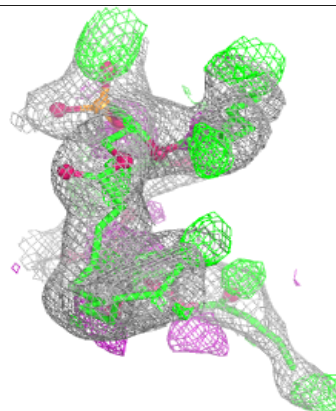
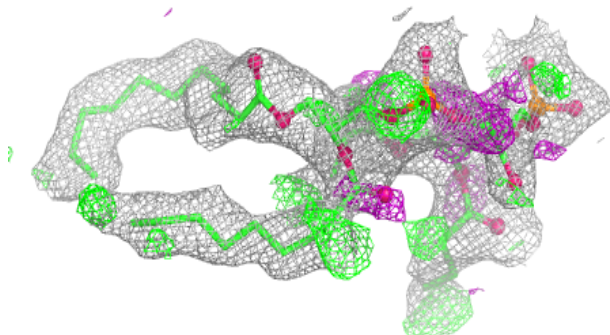
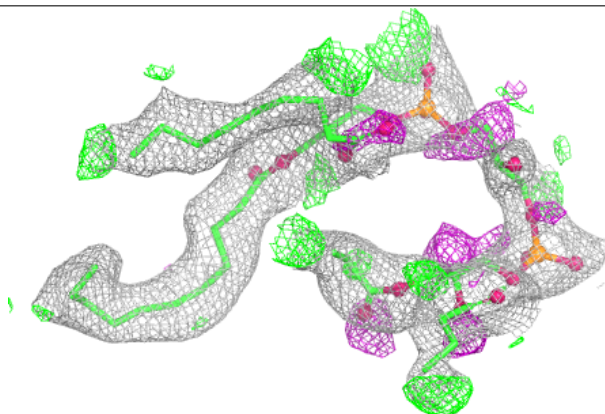


Electron density around CN3 D 4031:

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

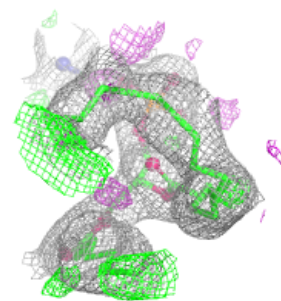
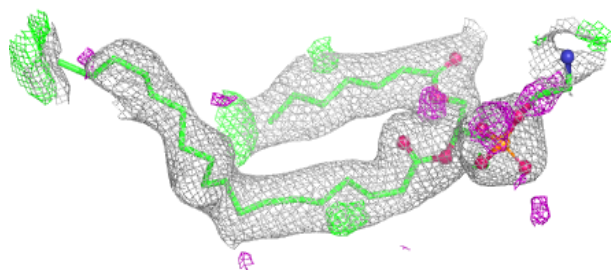
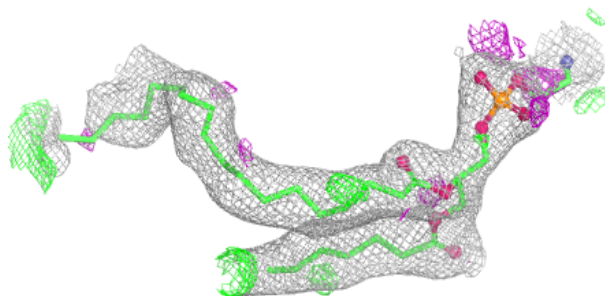
**Electron density around CN3 N 4131:**

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

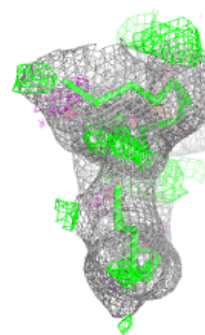
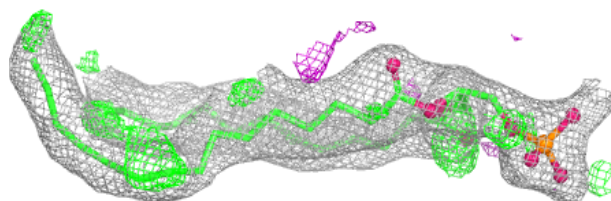
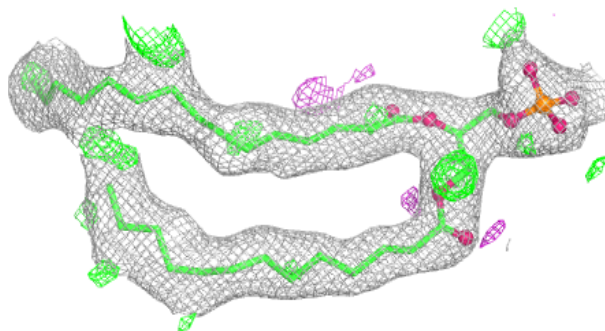


Electron density around 9PE N 4111:

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

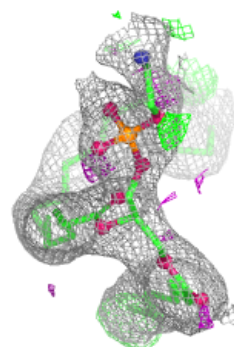
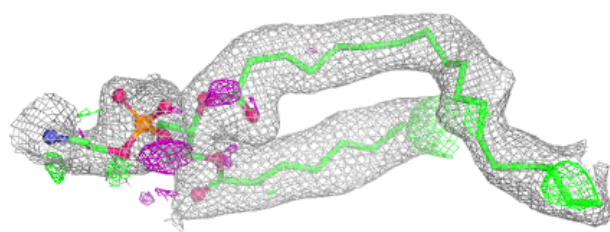
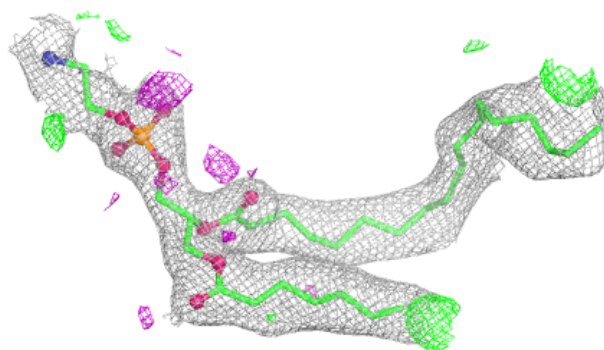
**Electron density around 6PH A 4013:**

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

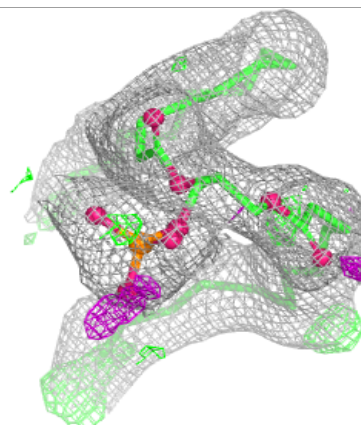
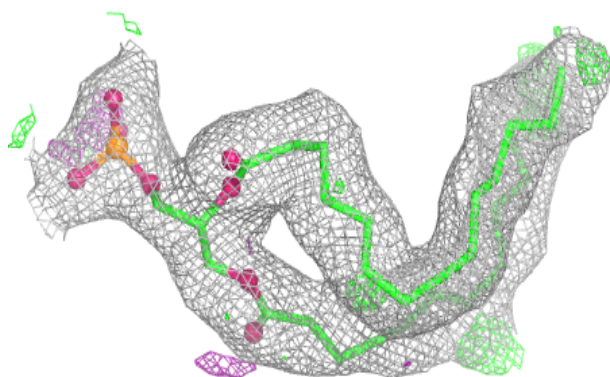
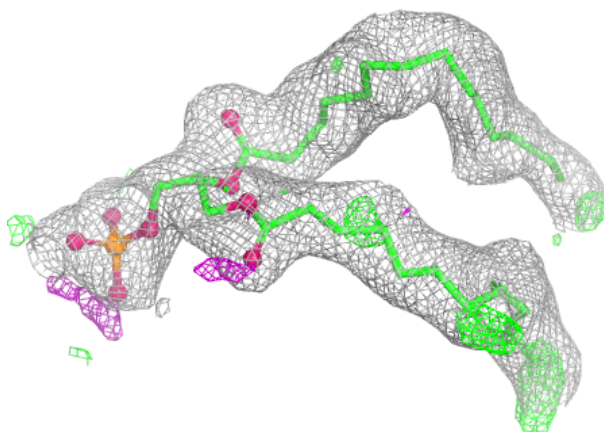


Electron density around 9PE C 4011:

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

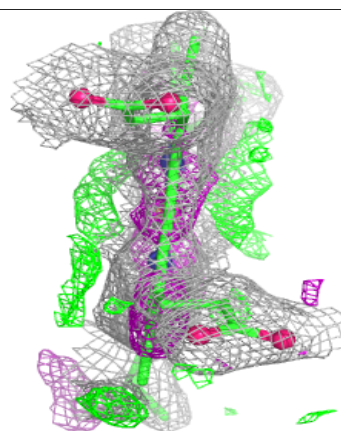
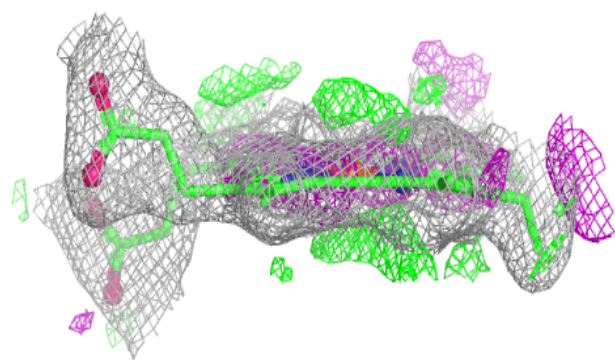
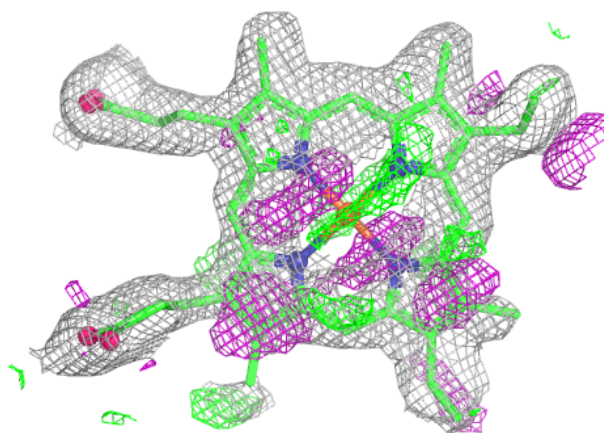
**Electron density around 7PH O 4114:**

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

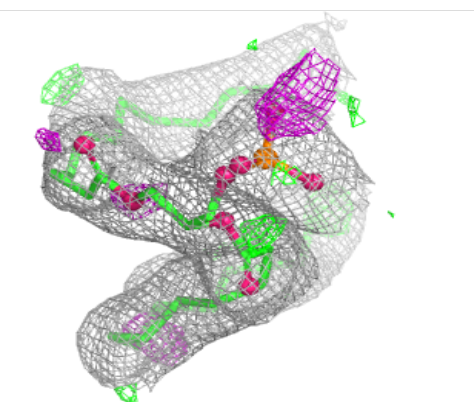
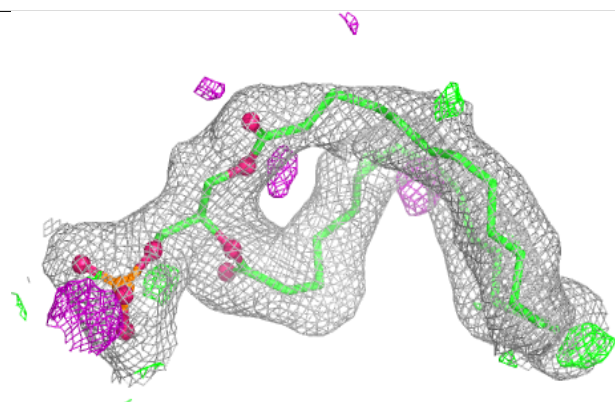
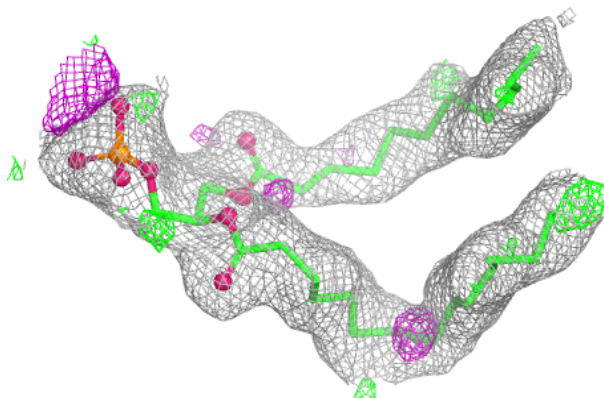


Electron density around HEM W 4026:

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

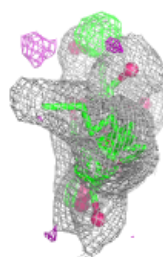
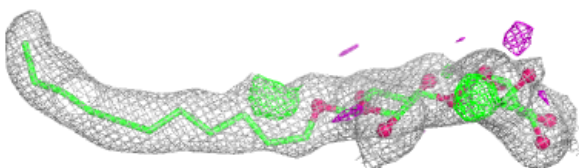
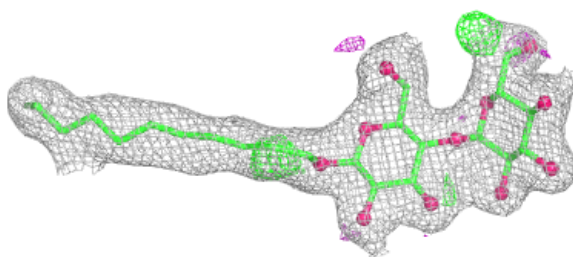
**Electron density around 7PH D 4014:**

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

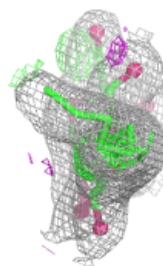
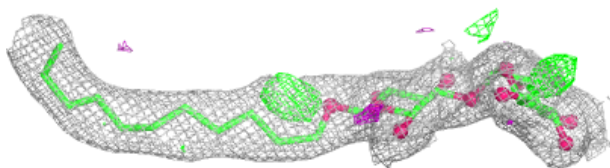
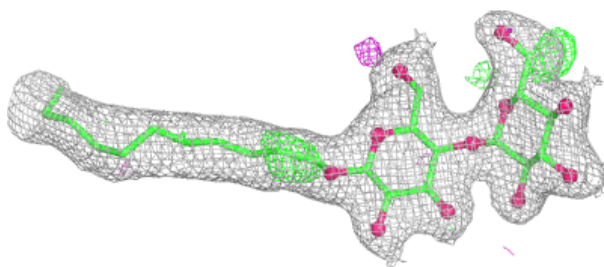


Electron density around UMQ A 4021:

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

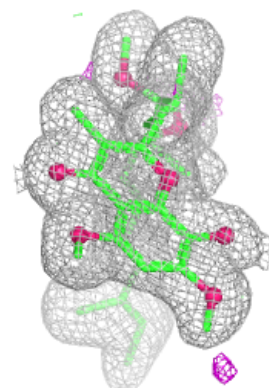
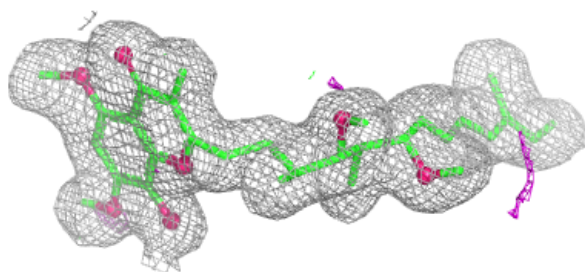
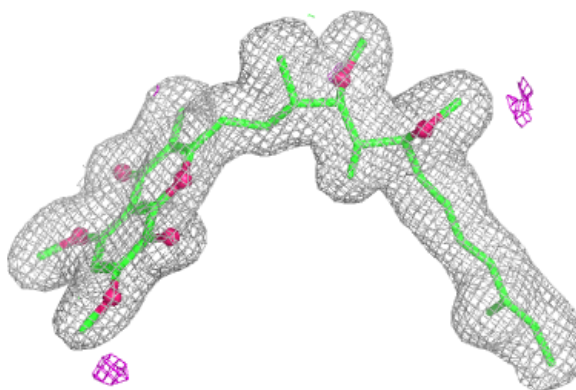
**Electron density around UMQ L 4121:**

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

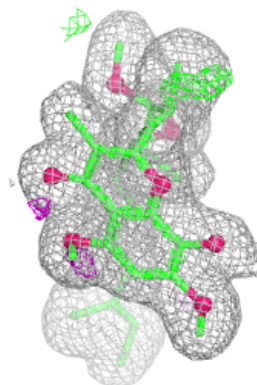
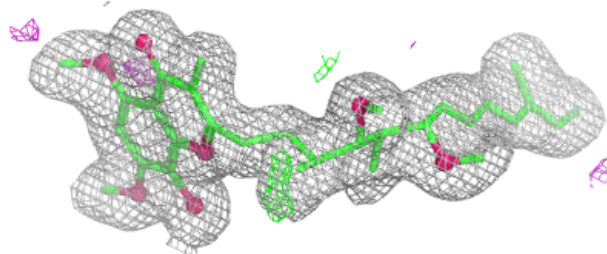
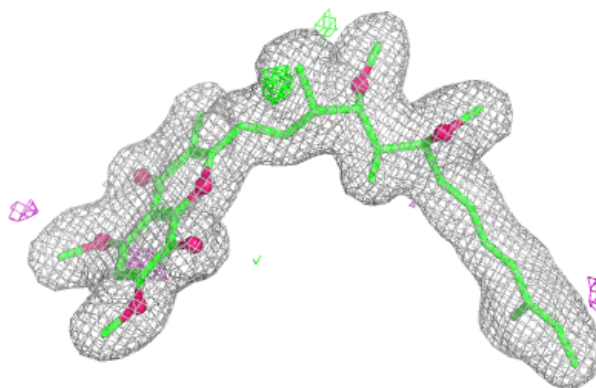


Electron density around SMA N 4025:

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

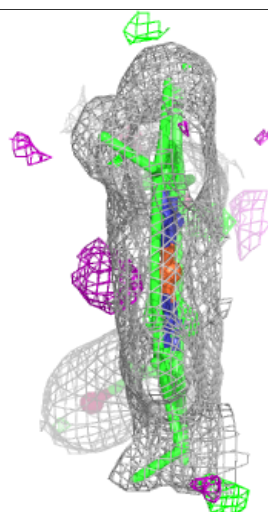
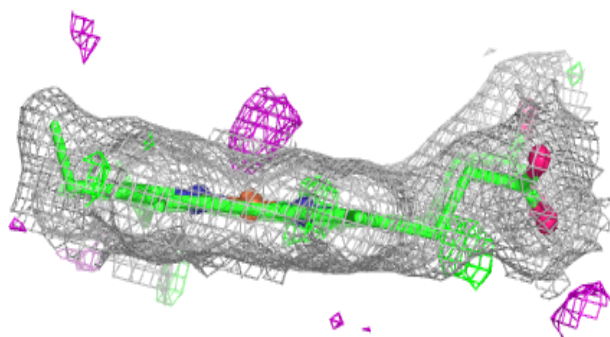
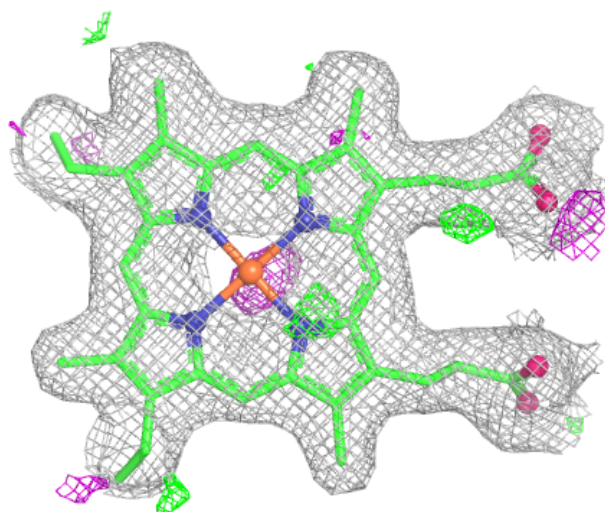
**Electron density around SMA C 4005:**

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



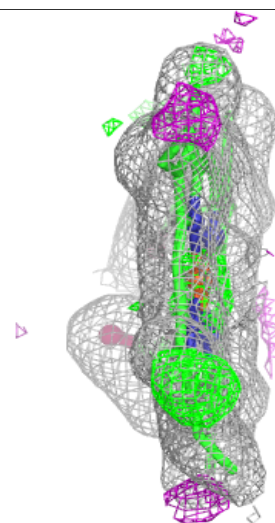
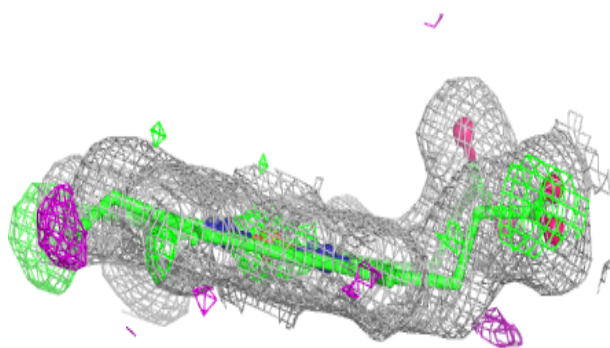
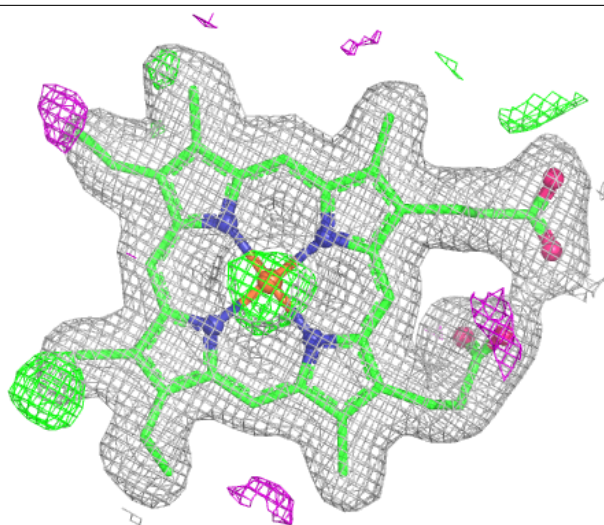
Electron density around HEM D 4003:

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



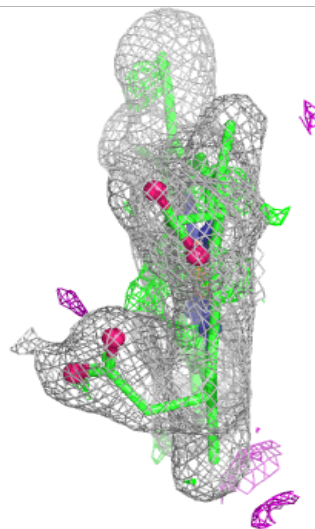
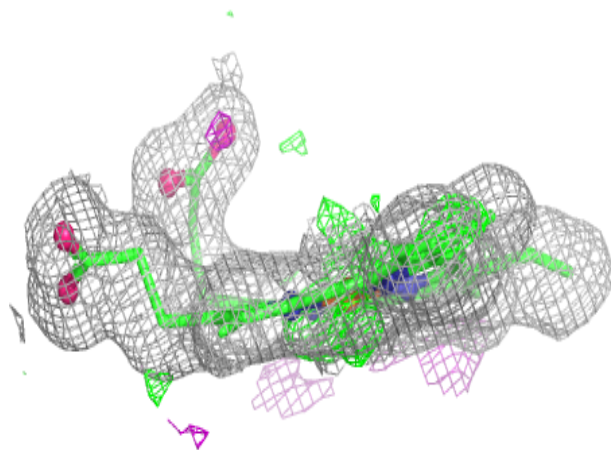
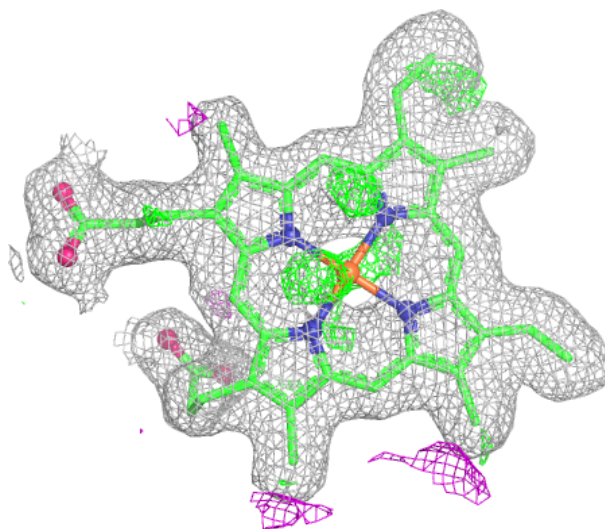
Electron density around HEM N 4021:

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



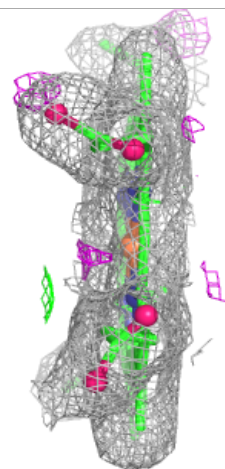
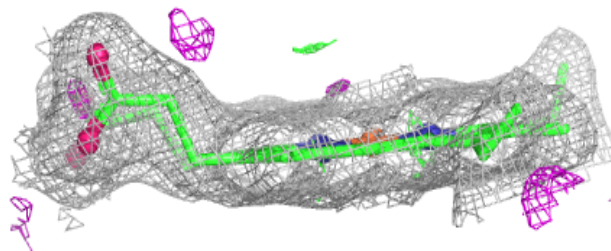
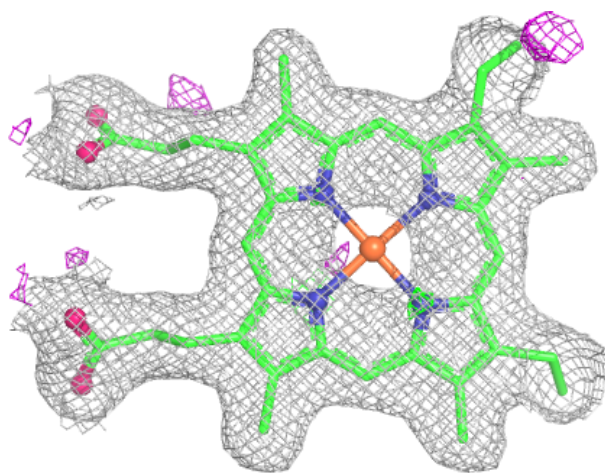
Electron density around HEM N 4022:

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



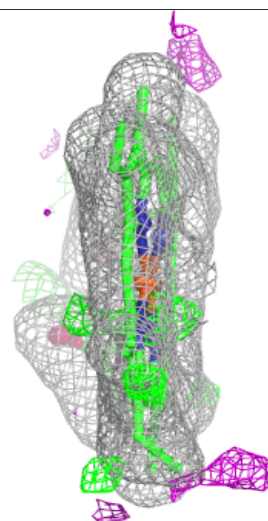
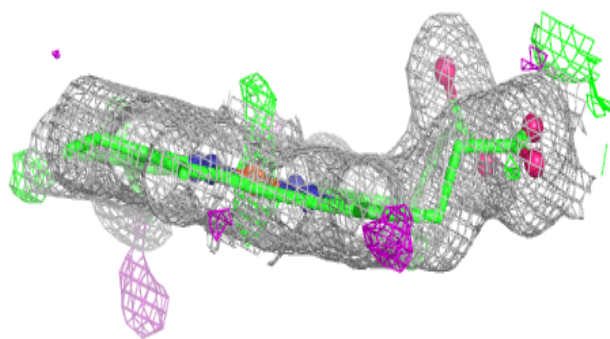
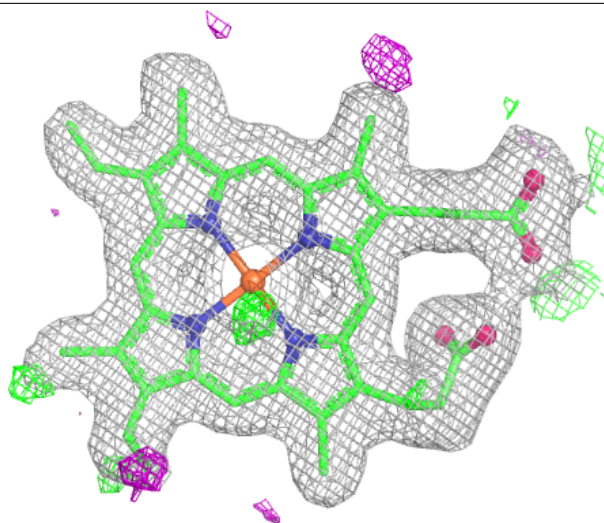
Electron density around HEM O 4023:

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



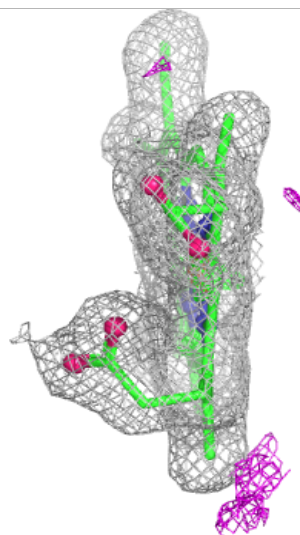
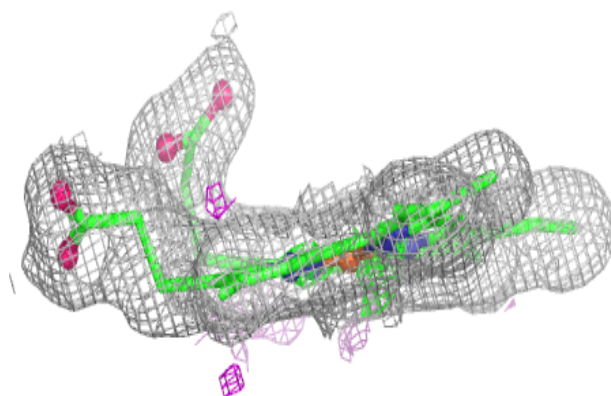
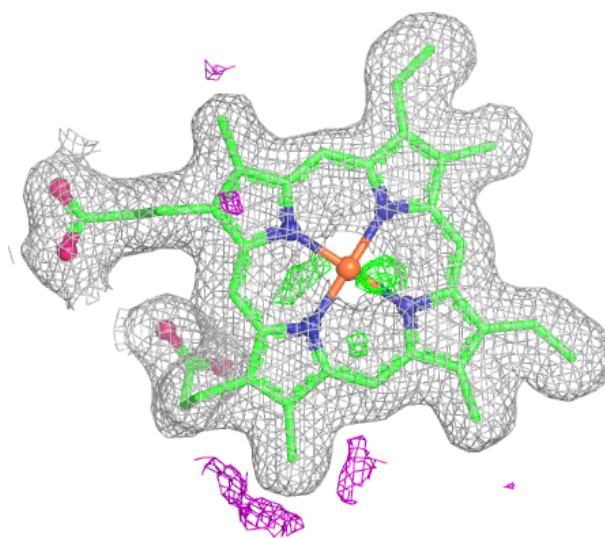
Electron density around HEM C 4001:

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



Electron density around HEM 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.