wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 06:39 AM EDT

PDB ID	:	2FBW
Title	:	Avian respiratory complex II with carboxin bound
Authors	:	Huang, L.S.; Sun, G.; Cobessi, D.; Wang, A.C.; Shen, J.T.; Tung, E.Y.; Anderson, V.E.; Berry, E.A.
Deposited on	:	2005-12-10
Resolution	:	2.06 Å(reported)

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

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

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

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

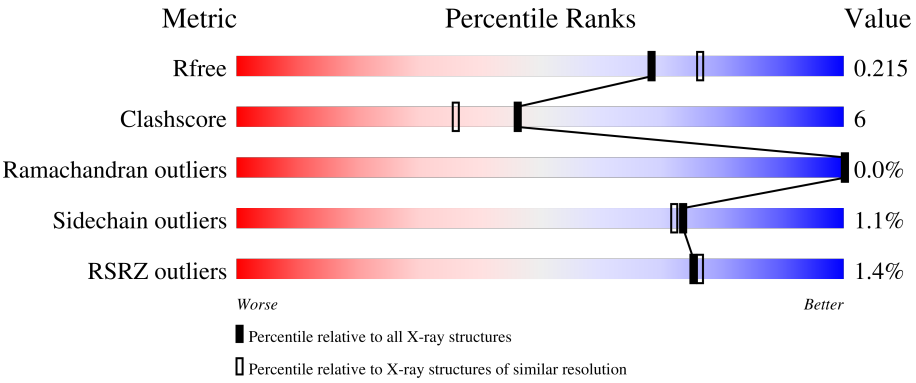
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.06 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	621	87% 12%
1	N	621	86% 12%
2	B	252	87% 8% 5%
2	O	252	86% 10%
3	C	140	86% 13%

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Mol	Chain	Length	Quality of chain
3	P	140	4% 84% 14%
4	D	103	4% 83% 16%
4	Q	103	11% 80% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	Y3P	A	1002	-	X	X	-
9	UNL	A	1368	-	-	X	-
9	UNL	B	1185	-	-	-	X
9	UNL	C	243	-	-	-	X
9	UNL	D	224	-	-	-	X
9	UNL	N	1388	-	-	-	X
9	UNL	N	1417[A]	-	-	-	X
9	UNL	N	1417[B]	-	-	-	X
9	UNL	O	1200	-	-	-	X
9	UNL	P	252	-	-	-	X
9	UNL	P	253	-	-	-	X
9	UNL	Q	213	-	-	-	X
9	UNL	Q	218	-	-	-	X

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 19296 atoms, of which 4 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 Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	1	4	0
			4737	2963	850	895	29			
1	N	612	Total	C	N	O	S	2	4	0
			4733	2962	847	895	29			

- Molecule 2 is a protein called Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	1	2	0
			1944	1228	331	363	22			
2	O	241	Total	C	N	O	S	0	2	0
			1953	1234	333	364	22			

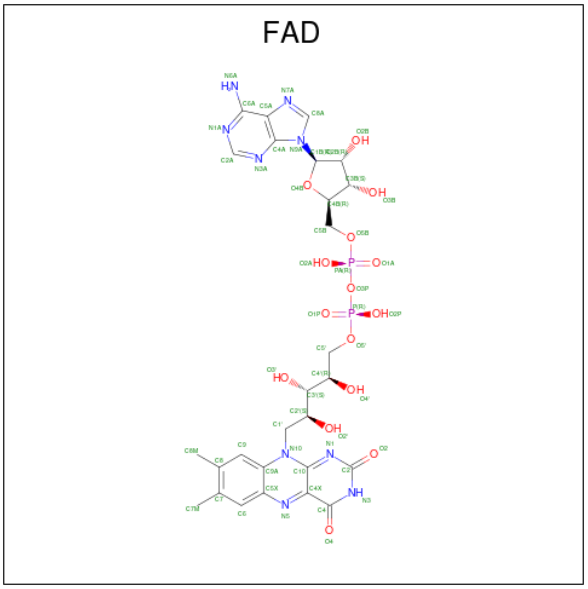
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b560 subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	139	Total	C	N	O	S	0	1	0
			1083	712	179	187	5			
3	P	139	Total	C	N	O	S	0	1	0
			1083	712	179	187	5			

- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

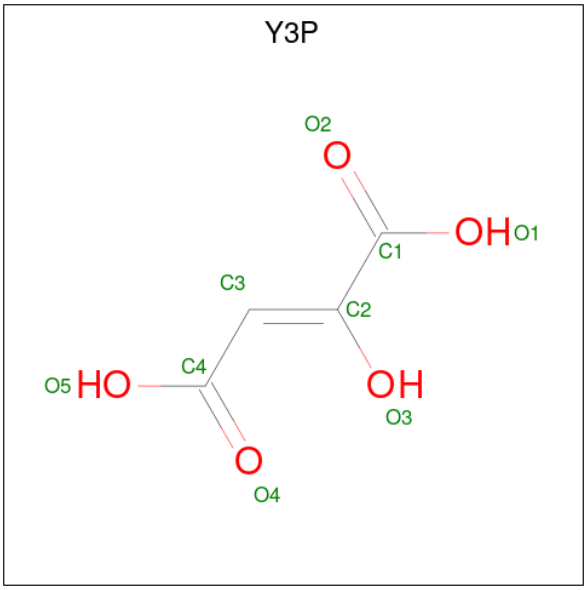
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	101	Total	C	N	O	S	0	1	0
			767	505	122	137	3			
4	Q	101	Total	C	N	O	S	0	0	0
			766	505	121	137	3			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	N	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is ({Z})-2-oxidanylbut-2-enedioic acid (three-letter code: Y3P) (formula: $C_4H_4O_5$) (labeled as "Ligand of Interest" by depositor).

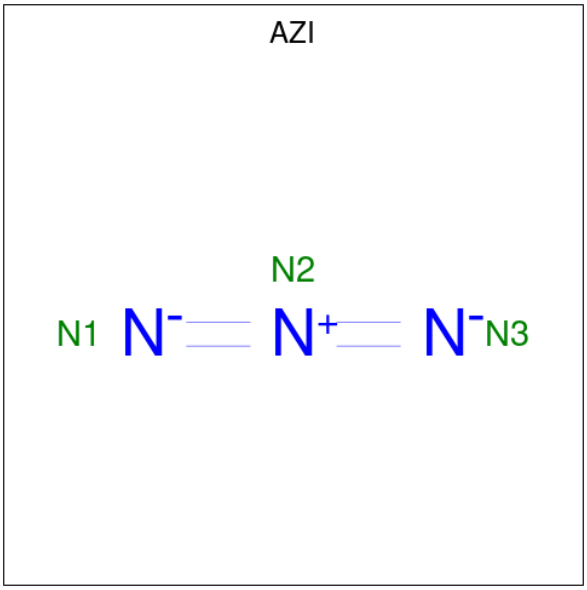


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 11 4 2 5	0	0
6	N	1	Total C H O 11 4 2 5	0	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0
7	N	1	Total K 1 1	0	0

- Molecule 8 is AZIDE ION (three-letter code: AZI) (formula: N_3).

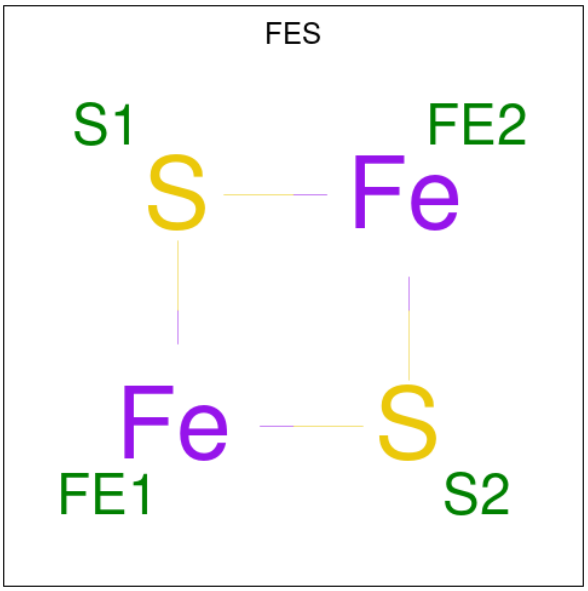


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total N 3 3	0	0
8	B	1	Total N 3 3	0	0
8	N	1	Total N 3 3	0	0

- Molecule 9 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

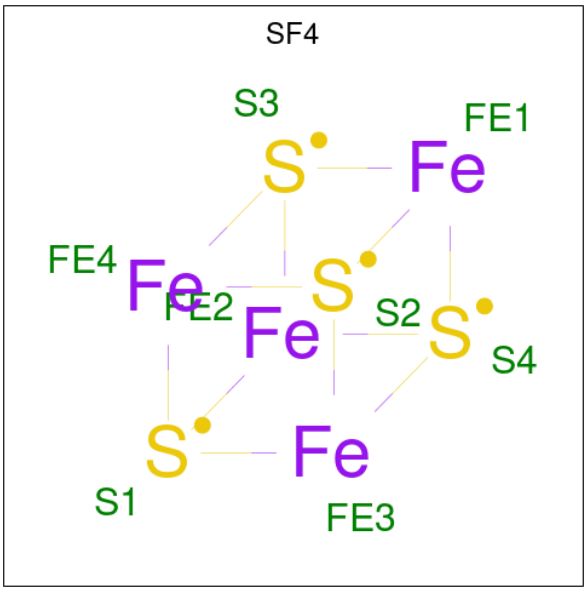
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	66	Total C N O S 129 30 15 83 1	0	8
9	B	43	Total C N O 77 11 15 51	0	5
9	C	19	Total C O 38 10 28	0	6
9	D	10	Total C O 52 29 23	0	1
9	N	64	Total C N O 142 31 21 90	0	11
9	O	36	Total C N O 84 20 12 52	0	9
9	P	9	Total C N O 43 26 3 14	0	0
9	Q	9	Total C O 74 45 29	0	1

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



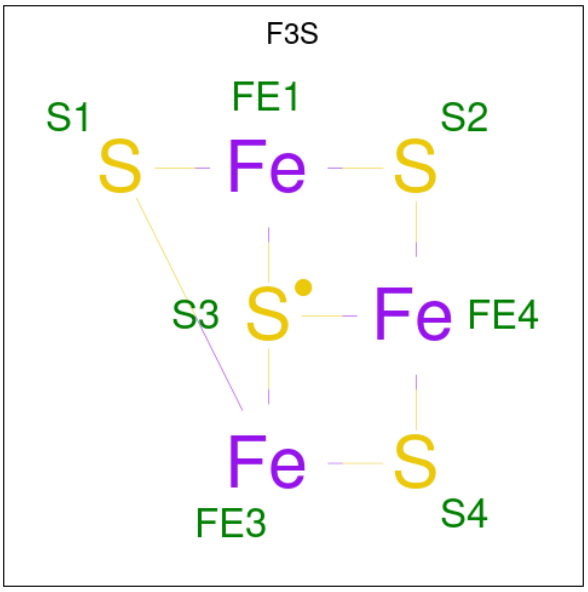
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Fe S 4 2 2	0	0
10	O	1	Total Fe S 4 2 2	0	0

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Fe S 8 4 4	0	0
11	O	1	Total Fe S 8 4 4	0	0

- Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total Fe S 7 3 4	0	0

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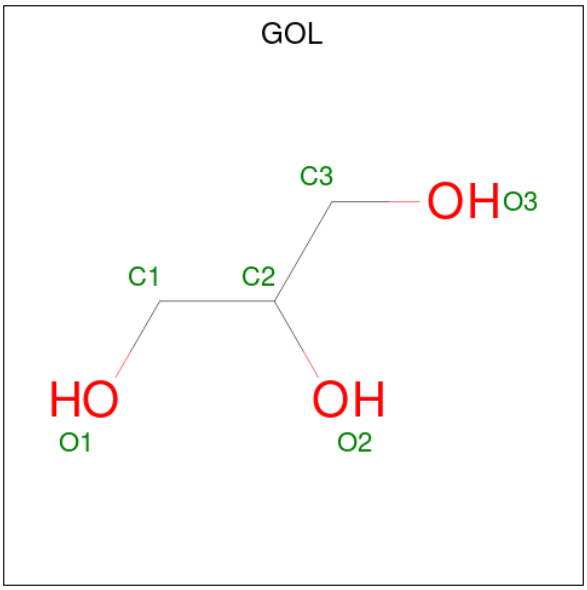
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	O	1	Total Fe S 7 3 4	0	0

- Molecule 13 is SODIUM ION (three-letter code: NA) (formula: Na).

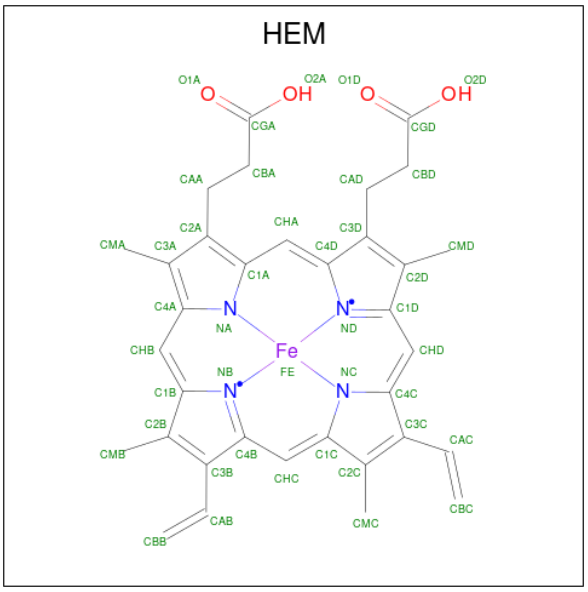
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total Na 1 1	0	0

- Molecule 14 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



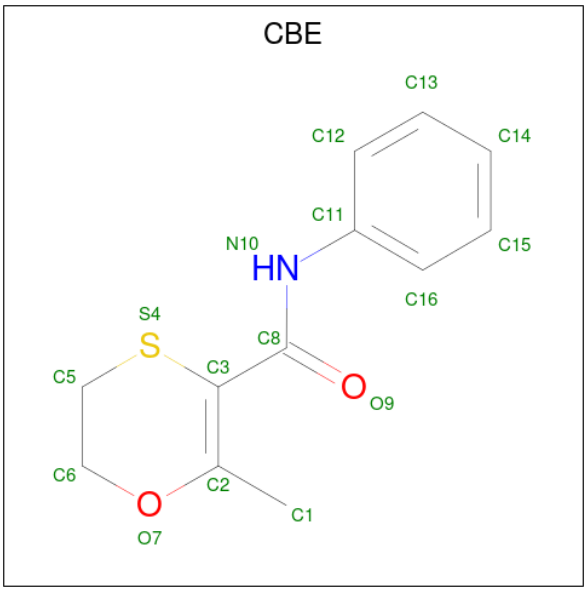
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total C O 6 3 3	0	0
14	N	1	Total C O 6 3 3	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	Fe	N	O	0	0
			41	32	1	4	4		
15	P	1	Total	C	Fe	N	O	0	0
			41	32	1	4	4		

- Molecule 16 is 2-METHYL-N-PHENYL-5,6-DIHYDRO-1,4-OXATHIINE-3-CARBOXAMIDE (three-letter code: CBE) (formula: $C_{12}H_{13}NO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

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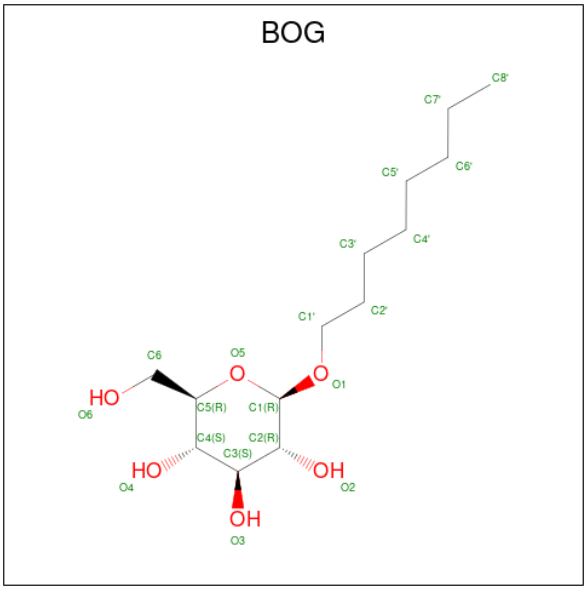
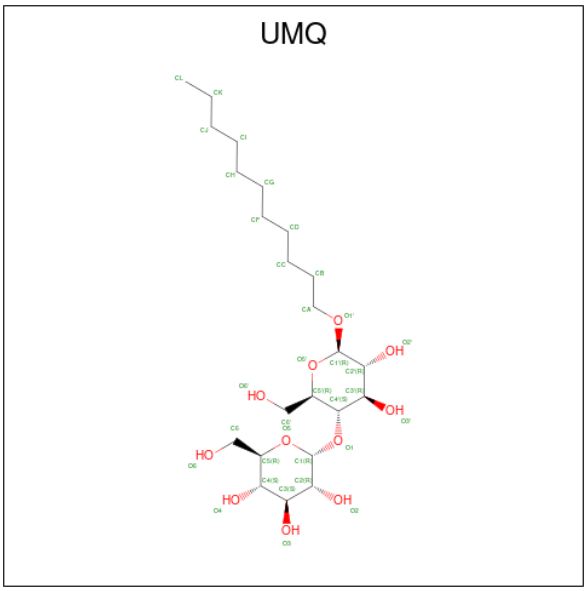
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	P	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

- Molecule 17 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	C	1	Total	C	O		0	0
			18	12	6			
17	D	1	Total	C	O		0	0
			17	11	6			
17	P	1	Total	C	O		0	0
			20	14	6			

- Molecule 18 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	P	1	Total C O 26 16 10	0	0

- Molecule 19 is water.

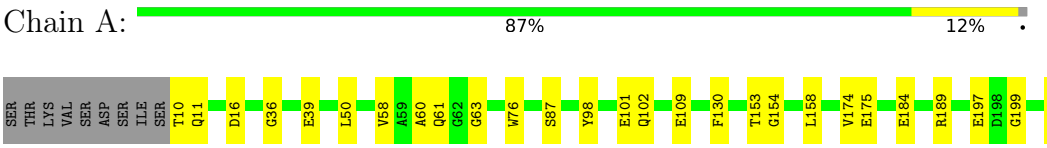
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	361	Total O 362 362	0	1
19	B	164	Total O 165 165	0	1
19	C	39	Total O 39 39	0	0
19	D	18	Total O 18 18	0	0
19	N	377	Total O 378 378	0	1
19	O	188	Total O 188 188	0	0
19	P	44	Total O 44 44	0	0
19	Q	12	Total O 12 12	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

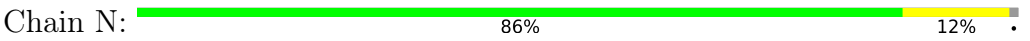
• Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

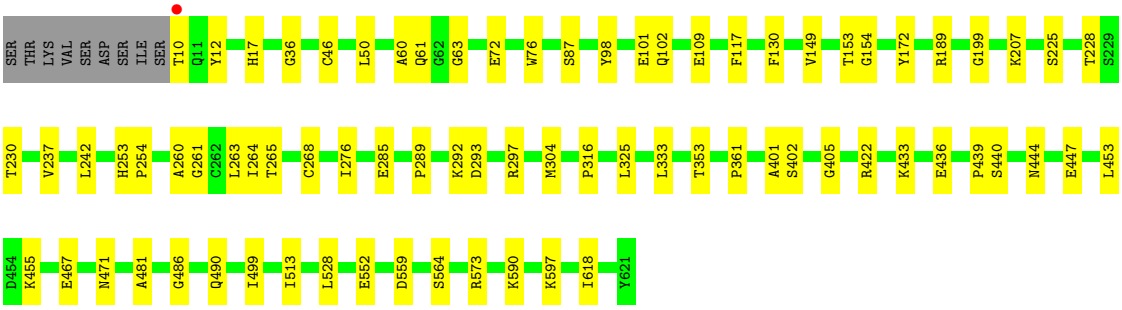
Chain A:



• Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

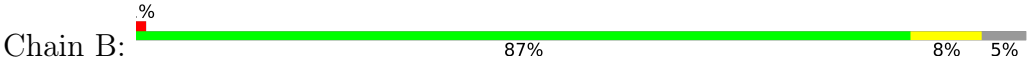
Chain N:

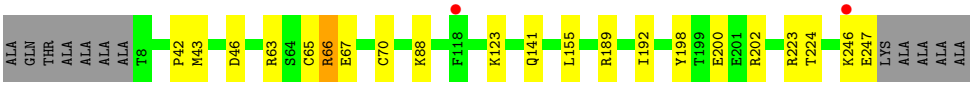




• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

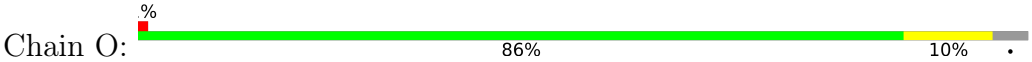
Chain B:



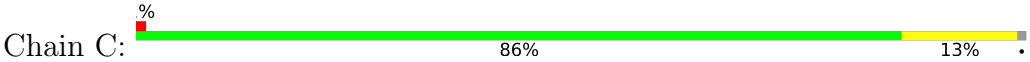


• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

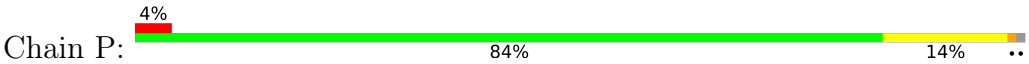
Chain O:

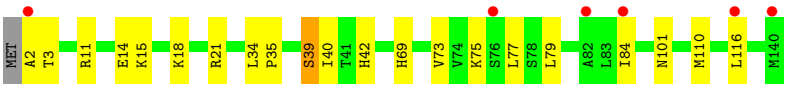


• Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial

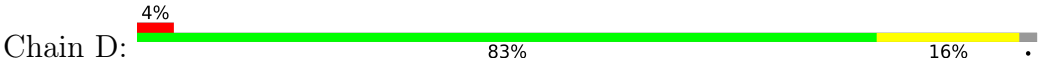


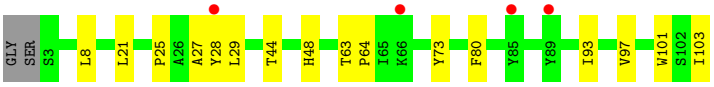
• Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial



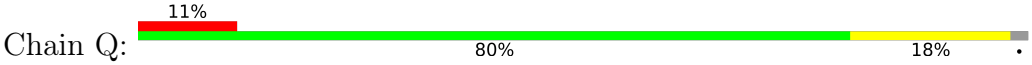


• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial





• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	118.70Å 200.75Å 67.63Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	64.09 – 2.06 64.09 – 2.06	Depositor EDS
% Data completeness (in resolution range)	85.2 (64.09-2.06) 85.1 (64.09-2.06)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.62 (at 2.05Å)	Xtriage
Refinement program	PHENIX dev_3150	Depositor
R, R_{free}	0.171 , 0.215 0.171 , 0.215	Depositor DCC
R_{free} test set	8237 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.287 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19296	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, UNL, BOG, UMQ, Y3P, NA, CBE, FAD, K, GOL, F3S, AZI, HEM, FES

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	0.40	0/4845	0.57	0/6559
1	N	0.40	0/4848	0.58	0/6564
2	B	0.40	0/1987	0.55	0/2678
2	O	0.38	0/1996	0.54	0/2689
3	C	0.30	0/1112	0.45	0/1511
3	P	0.30	0/1112	0.46	0/1511
4	D	0.28	0/798	0.41	0/1093
4	Q	0.27	0/789	0.40	0/1082
All	All	0.37	0/17487	0.54	0/23687

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4737	0	4614	57	0
1	N	4733	0	4616	56	0
2	B	1944	0	1937	28	0
2	O	1953	0	1950	26	0
3	C	1083	0	1125	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	1083	0	1125	19	0
4	D	767	0	752	9	0
4	Q	766	0	761	14	0
5	A	53	0	29	3	0
5	N	53	0	29	4	0
6	A	9	2	0	4	0
6	N	9	2	0	2	0
7	A	1	0	0	0	0
7	N	1	0	0	0	0
8	A	3	0	0	0	0
8	B	3	0	0	0	0
8	N	3	0	0	0	0
9	A	129	0	0	9	0
9	B	77	0	0	4	0
9	C	38	0	0	3	0
9	D	52	0	0	1	0
9	N	142	0	0	7	0
9	O	84	0	0	3	0
9	P	43	0	0	0	0
9	Q	74	0	0	2	0
10	B	4	0	0	0	0
10	O	4	0	0	0	0
11	B	8	0	0	0	0
11	O	8	0	0	0	0
12	B	7	0	0	0	0
12	O	7	0	0	0	0
13	B	1	0	0	0	0
14	B	6	0	8	0	0
14	N	6	0	8	3	0
15	C	41	0	24	1	0
15	P	41	0	24	2	0
16	C	16	0	13	1	0
16	P	16	0	13	2	0
17	C	18	0	21	0	0
17	D	17	0	19	2	0
17	P	20	0	28	4	0
18	P	26	0	25	7	0
19	A	362	0	0	7	0
19	B	165	0	0	0	0
19	C	39	0	0	0	0
19	D	18	0	0	0	0
19	N	378	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	O	188	0	0	3	0
19	P	44	0	0	0	0
19	Q	12	0	0	0	0
All	All	19292	4	17121	221	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 6.

The worst 5 of 221 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)
1:N:189:ARG:HD3	1:N:439:PRO:HB2	1.34	1.07
1:A:189:ARG:HD3	1:A:439:PRO:HB2	1.37	1.07
1:A:223:CYS:O	2:B:66[B]:ARG:NH2	2.02	0.93
1:A:218[A]:ARG:HH22	2:B:66[A]:ARG:HH21	1.19	0.90
1:A:297:ARG:HH22	6:A:1002:Y3P:C3	1.86	0.88

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	614/621 (99%)	594 (97%)	20 (3%)	0	100	100
1	N	614/621 (99%)	596 (97%)	18 (3%)	0	100	100
2	B	240/252 (95%)	234 (98%)	6 (2%)	0	100	100
2	O	241/252 (96%)	234 (97%)	6 (2%)	1 (0%)	34	25
3	C	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
3	P	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
4	D	100/103 (97%)	99 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
All	All	2184/2232 (98%)	2128 (97%)	55 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	247	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	496/506 (98%)	494 (100%)	2 (0%)	91	91
1	N	497/506 (98%)	493 (99%)	4 (1%)	81	81
2	B	218/219 (100%)	212 (97%)	6 (3%)	43	37
2	O	219/219 (100%)	215 (98%)	4 (2%)	59	55
3	C	118/118 (100%)	118 (100%)	0	100	100
3	P	118/118 (100%)	117 (99%)	1 (1%)	81	81
4	D	79/79 (100%)	77 (98%)	2 (2%)	47	41
4	Q	78/79 (99%)	76 (97%)	2 (3%)	46	40
All	All	1823/1844 (99%)	1802 (99%)	21 (1%)	73	69

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	63	ARG
2	O	224	THR
4	Q	101	TRP
3	P	39	SER
2	O	189	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
2	O	174	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 323 ligands modelled in this entry, 3 are monoatomic and 297 are unknown - leaving 23 for Mogul analysis.

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	$\#\|Z\| > 2$
17	BOG	C	203	-	18,18,20	0.54	0	23,23,25	0.67	0
17	BOG	D	201	-	17,17,20	0.68	1 (5%)	22,22,25	0.73	1 (4%)
15	HEM	P	201	4,3	40,48,50	1.28	4 (10%)	46,80,82	1.39	6 (13%)
14	GOL	N	1005	-	5,5,5	0.07	0	5,5,5	0.28	0
12	F3S	B	1003	2	0,9,9	-	-	-		
12	F3S	O	1003	2	0,9,9	-	-	-		
6	Y3P	N	1002	-	8,8,8	2.82	5 (62%)	9,10,10	1.17	0
8	AZI	B	1005	-	0,2,2	-	-	0,1,1	-	-
5	FAD	A	1001	1	53,58,58	0.84	0	68,89,89	0.89	1 (1%)
10	FES	B	1001	2	0,4,4	-	-	-		
11	SF4	O	1002	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	Y3P	A	1002	-	8,8,8	2.76	5 (62%)	9,10,10	1.62	3 (33%)
17	BOG	P	204	-	20,20,20	0.50	0	25,25,25	0.69	1 (4%)
8	AZI	N	1004	-	0,2,2	-	-	0,1,1	-	-
18	UMQ	P	203	-	27,27,35	0.24	0	37,37,46	0.46	0
10	FES	O	1001	2	0,4,4	-	-	-		
8	AZI	A	1004	-	0,2,2	-	-	0,1,1	-	-
16	CBE	C	202	-	16,17,17	2.07	4 (25%)	16,22,22	2.00	4 (25%)
5	FAD	N	1001	1	53,58,58	1.01	5 (9%)	68,89,89	0.89	3 (4%)
11	SF4	B	1002	2	0,12,12	-	-	-		
15	HEM	C	201	4,3	40,48,50	1.29	3 (7%)	46,80,82	1.44	7 (15%)
16	CBE	P	202	-	16,17,17	2.20	3 (18%)	16,22,22	1.99	3 (18%)
14	GOL	B	1006	-	5,5,5	0.08	0	5,5,5	0.32	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
17	BOG	C	203	-	-	4/9/29/31	0/1/1/1
17	BOG	D	201	-	-	1/8/28/31	0/1/1/1
15	HEM	P	201	4,3	-	1/10/50/54	-
14	GOL	N	1005	-	-	0/4/4/4	-
12	F3S	B	1003	2	-	-	0/3/3/3
12	F3S	O	1003	2	-	-	0/3/3/3
6	Y3P	N	1002	-	-	4/8/8/8	-
5	FAD	A	1001	1	-	7/30/50/50	0/6/6/6
10	FES	B	1001	2	-	-	0/1/1/1
11	SF4	O	1002	2	-	-	0/6/5/5
6	Y3P	A	1002	-	-	4/8/8/8	-
17	BOG	P	204	-	-	1/11/31/31	0/1/1/1
18	UMQ	P	203	-	-	2/12/49/60	0/2/2/2
10	FES	O	1001	2	-	-	0/1/1/1
16	CBE	C	202	-	-	2/6/19/19	0/1/2/2
5	FAD	N	1001	1	-	6/30/50/50	0/6/6/6
11	SF4	B	1002	2	-	-	0/6/5/5
15	HEM	C	201	4,3	-	1/10/50/54	-
16	CBE	P	202	-	-	2/6/19/19	0/1/2/2
14	GOL	B	1006	-	-	0/4/4/4	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	202	CBE	O7-C2	6.84	1.46	1.37
16	C	202	CBE	O7-C2	5.97	1.44	1.37
6	N	1002	Y3P	C2-C1	5.66	1.55	1.48
6	A	1002	Y3P	C2-C1	5.59	1.55	1.48
16	C	202	CBE	C11-N10	-3.61	1.34	1.41

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	P	202	CBE	O7-C2-C1	6.78	117.48	109.32
16	C	202	CBE	O7-C2-C1	6.66	117.34	109.32
15	C	201	HEM	C4B-CHC-C1C	3.04	126.57	122.56
15	C	201	HEM	C1B-NB-C4B	2.98	108.15	105.07
15	P	201	HEM	C4B-CHC-C1C	2.89	126.37	122.56

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	FAD	N10-C1'-C2'-O2'
5	A	1001	FAD	N10-C1'-C2'-C3'
5	N	1001	FAD	N10-C1'-C2'-O2'
5	N	1001	FAD	N10-C1'-C2'-C3'
6	A	1002	Y3P	O1-C1-C2-O3

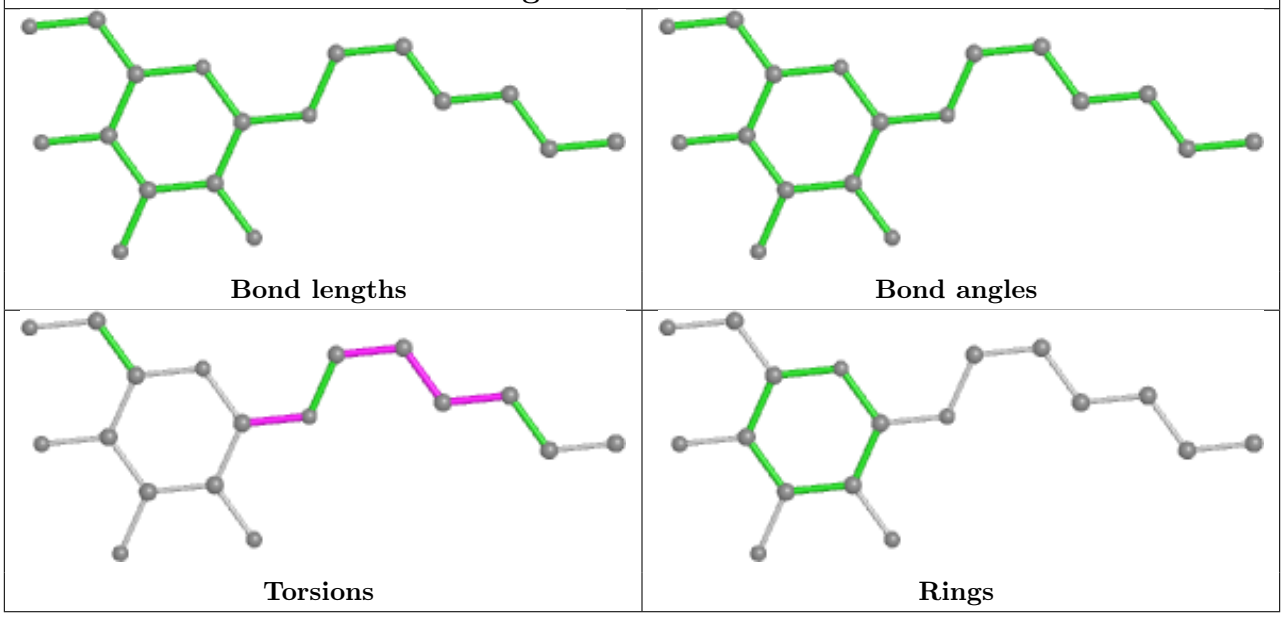
There are no ring outliers.

12 monomers are involved in 31 short contacts:

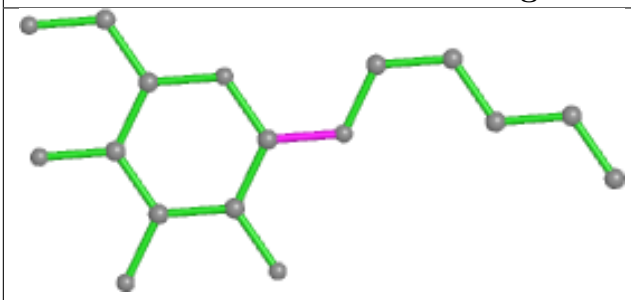
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	201	BOG	2	0
15	P	201	HEM	2	0
14	N	1005	GOL	3	0
6	N	1002	Y3P	2	0
5	A	1001	FAD	3	0
6	A	1002	Y3P	4	0
17	P	204	BOG	4	0
18	P	203	UMQ	7	0
16	C	202	CBE	1	0
5	N	1001	FAD	4	0
15	C	201	HEM	1	0
16	P	202	CBE	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

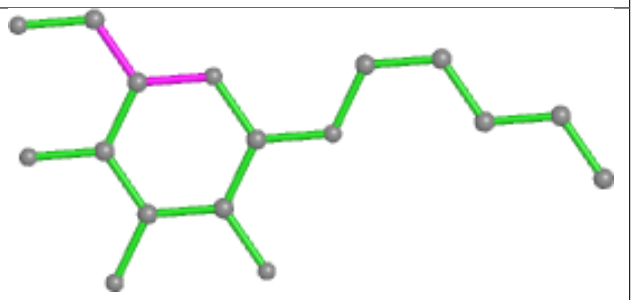
Ligand BOG C 203



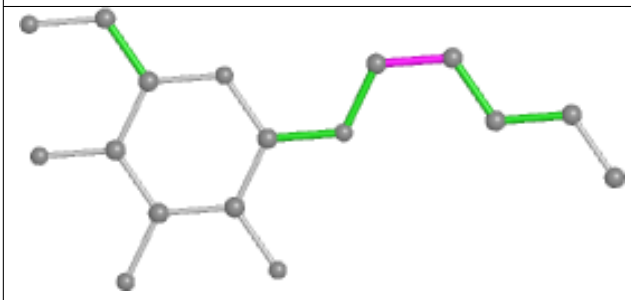
Ligand BOG D 201



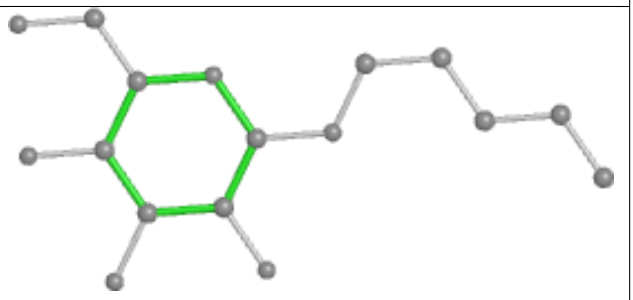
Bond lengths



Bond angles

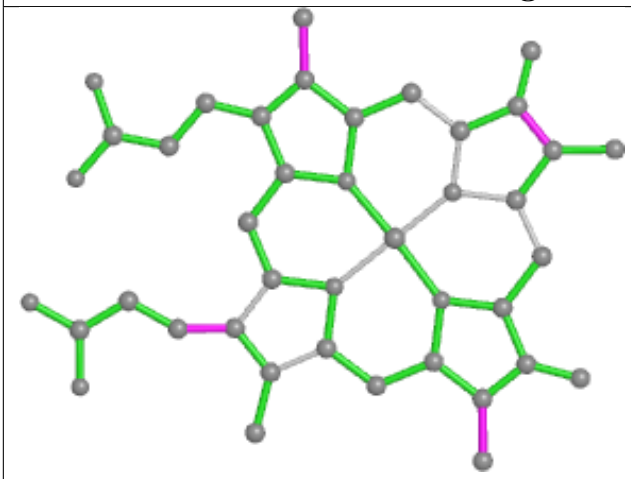


Torsions



Rings

Ligand HEM P 201



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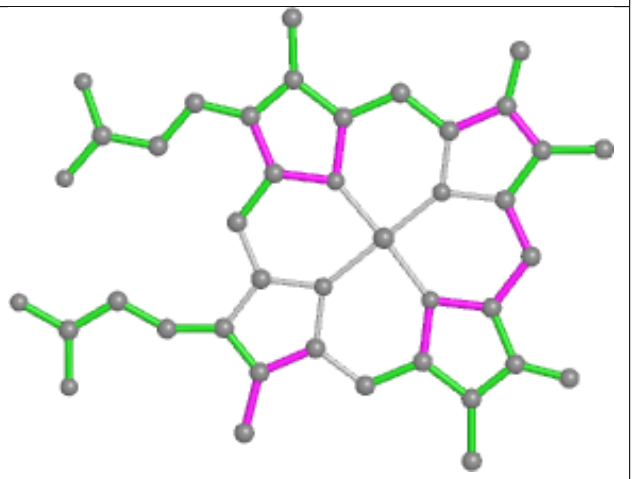

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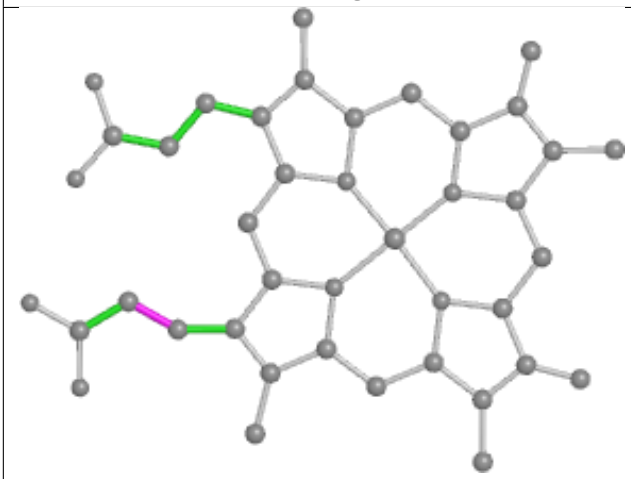

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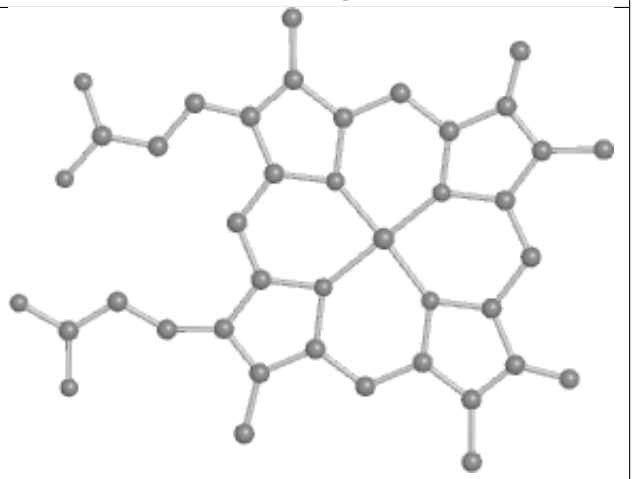
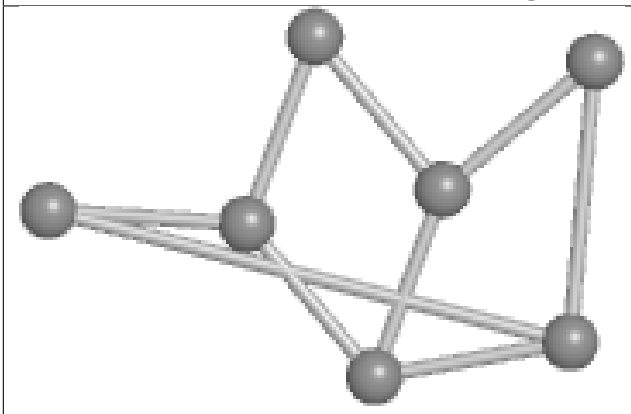


Rings

Ligand F3S B 1003



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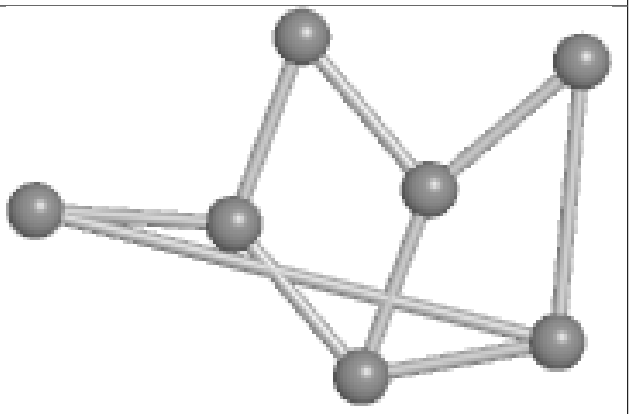
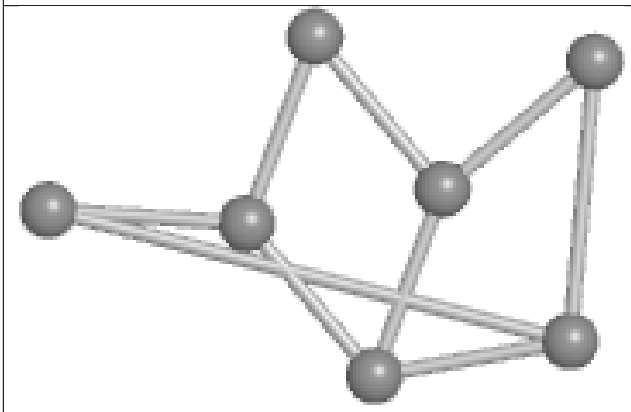


Bond angles



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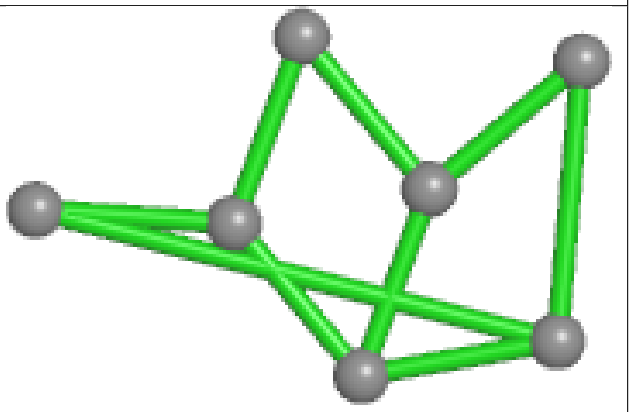
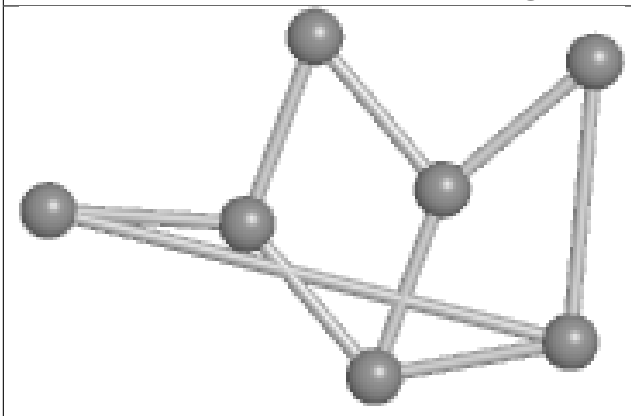
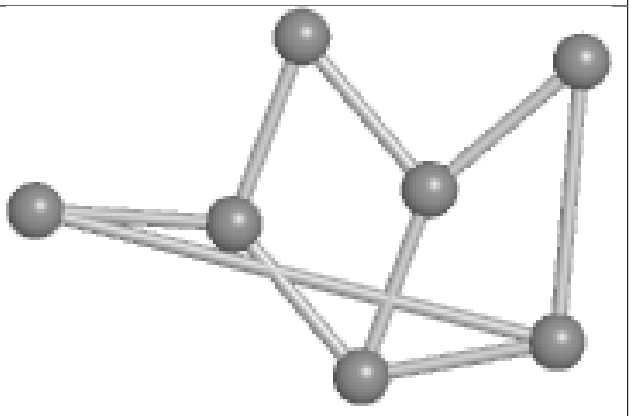


Rings

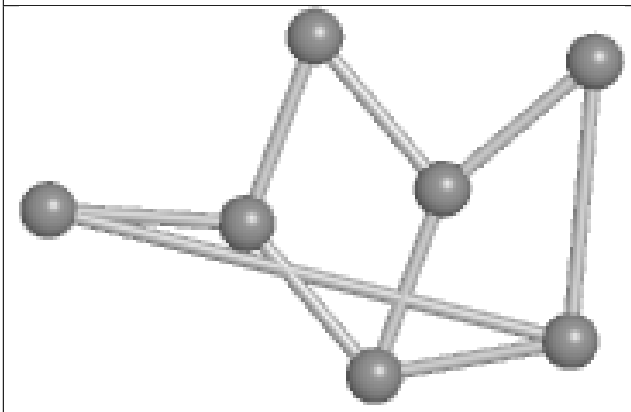
Ligand F3S O 1003



Bond lengths



Bond angles



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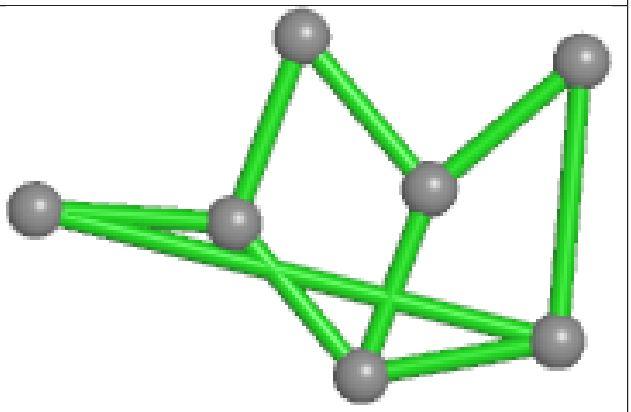
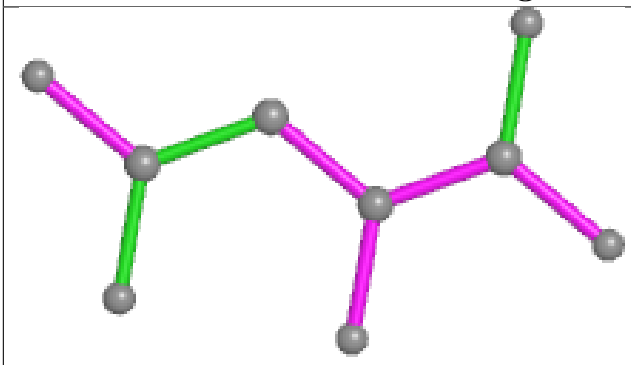
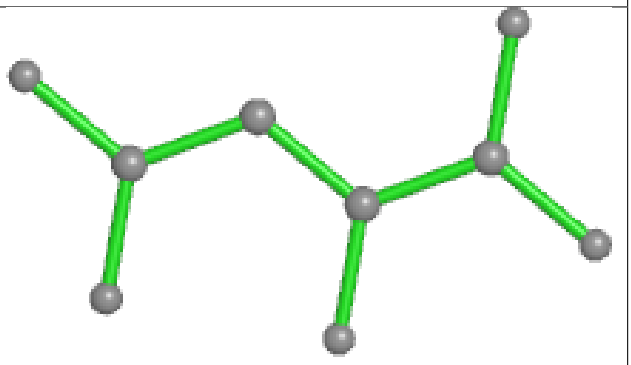


Rings

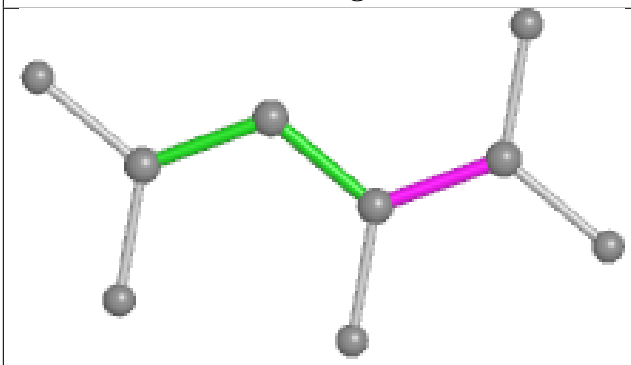
Ligand Y3P N 1002



Bond lengths



Bond angles



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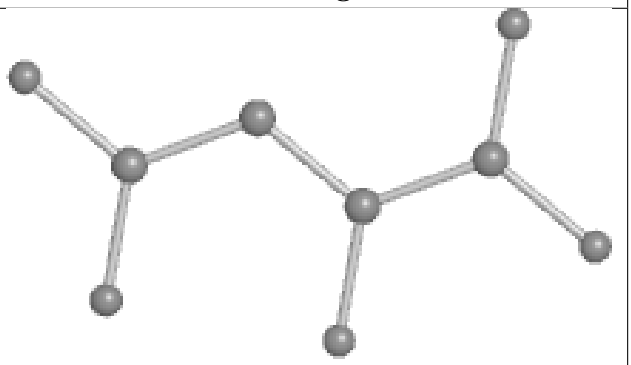
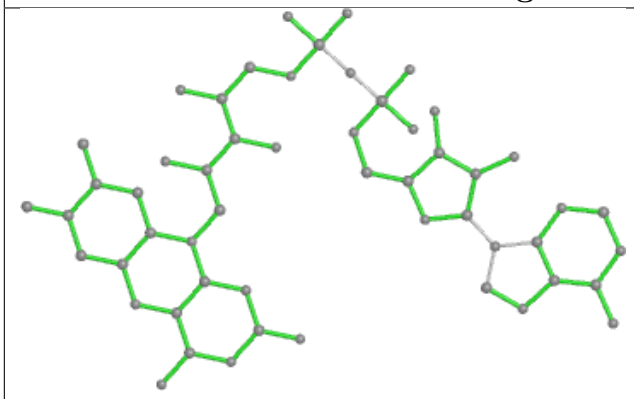
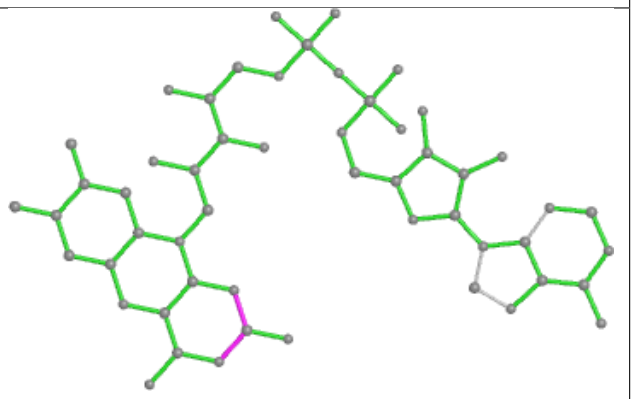


Rings

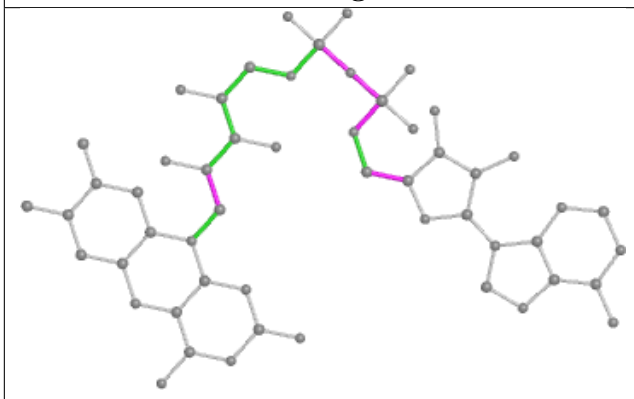
Ligand FAD A 1001



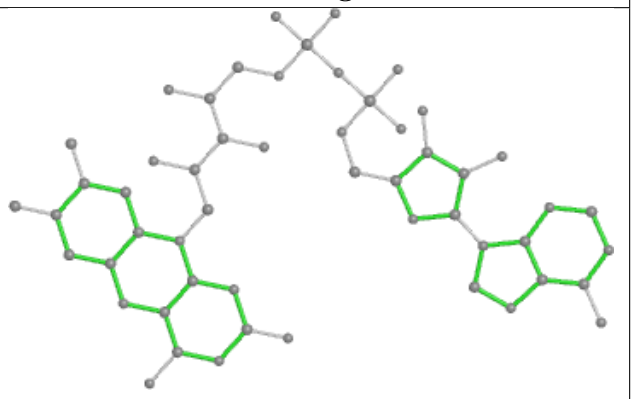
Bond lengths



Bond angles

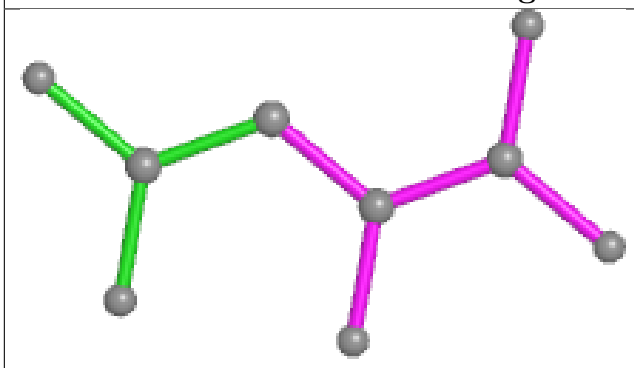


Torsions

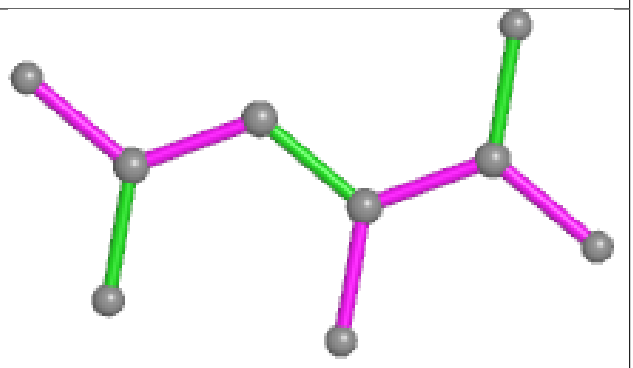


Rings

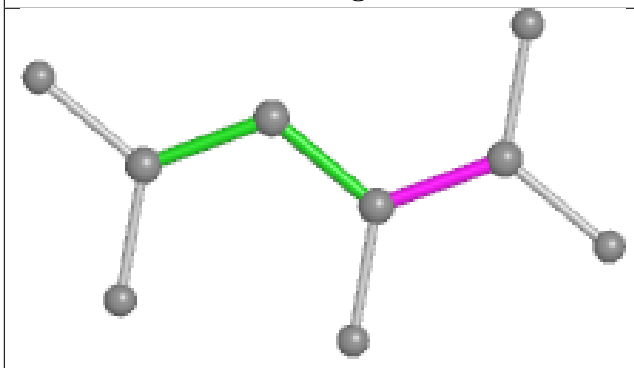
Ligand Y3P A 1002



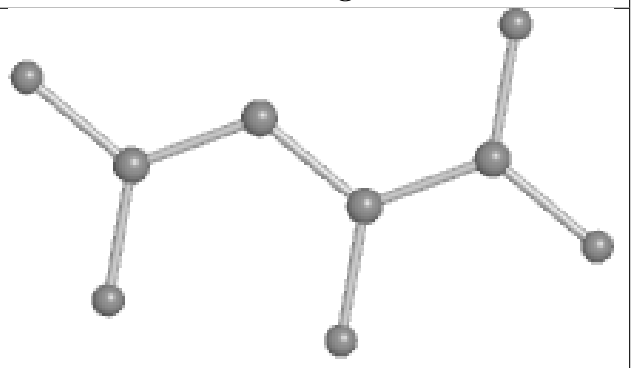
Bond lengths



Bond angles

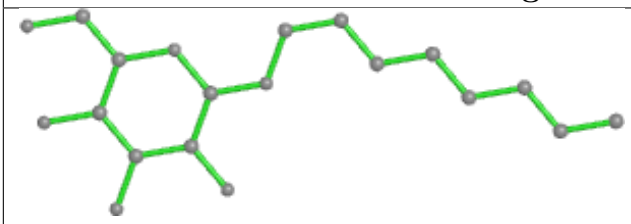


Torsions

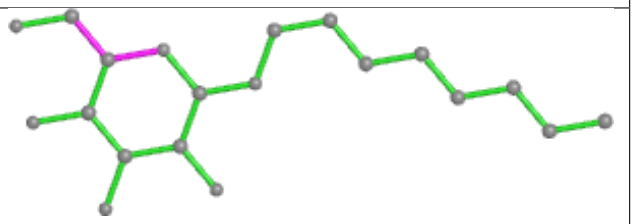


Rings

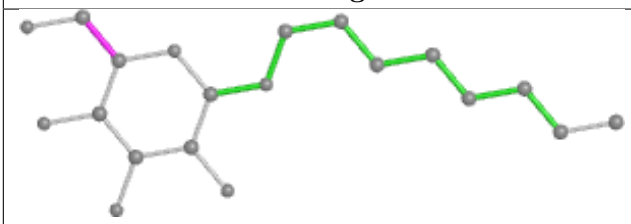
Ligand BOG P 204



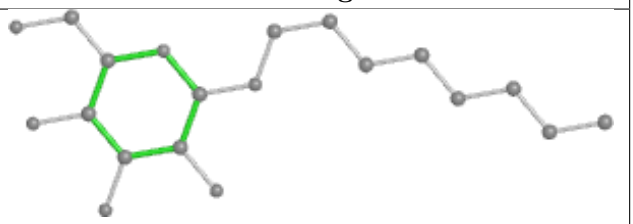
Bond lengths



Bond angles

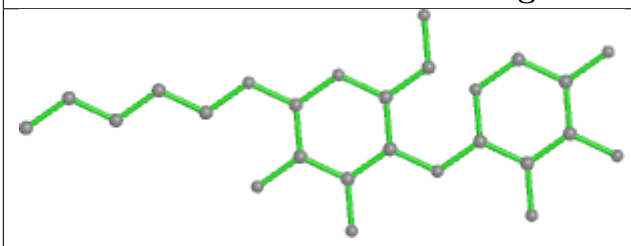


Torsions

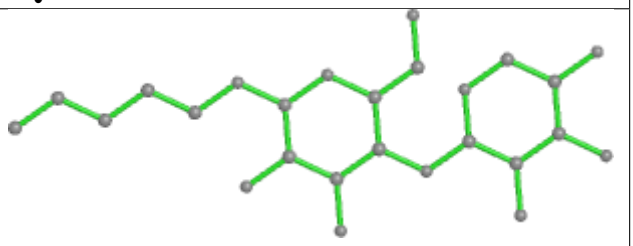


Rings

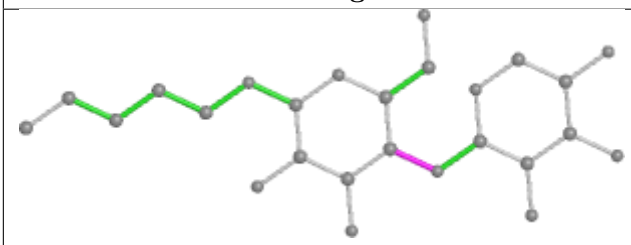
Ligand UMQ P 203



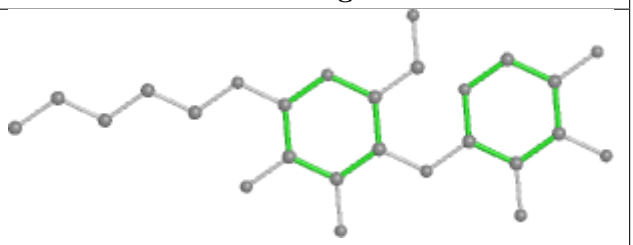
Bond lengths



Bond angles

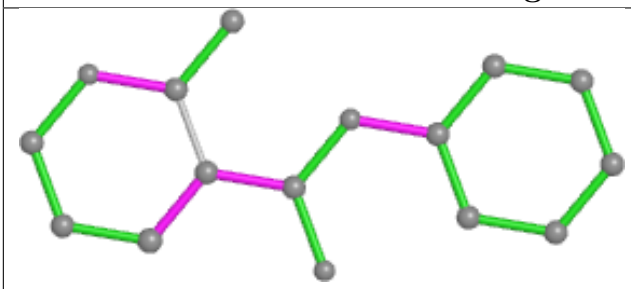


Torsions

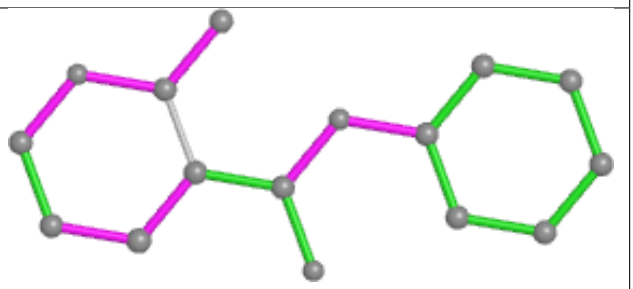


Rings

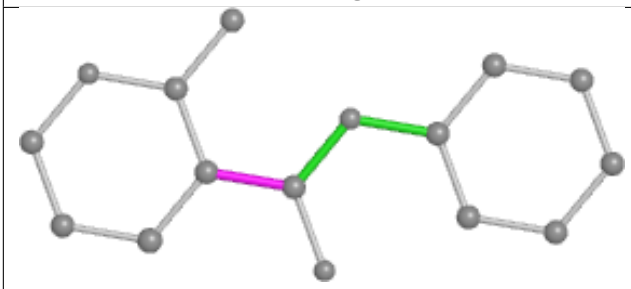
Ligand CBE C 202



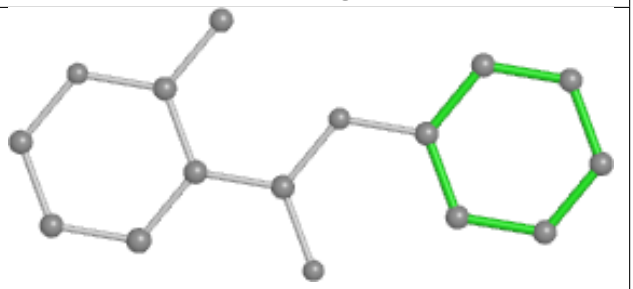
Bond lengths



Bond angles

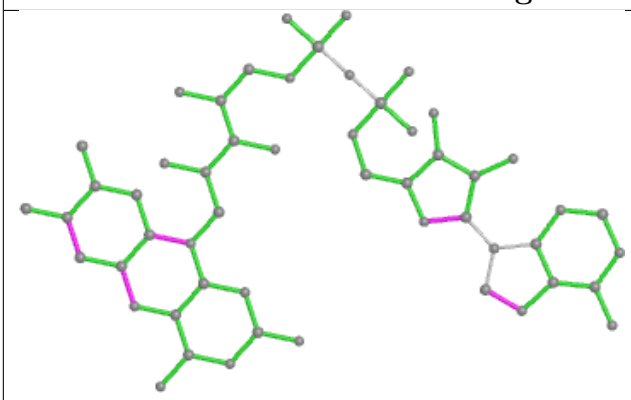


Torsions

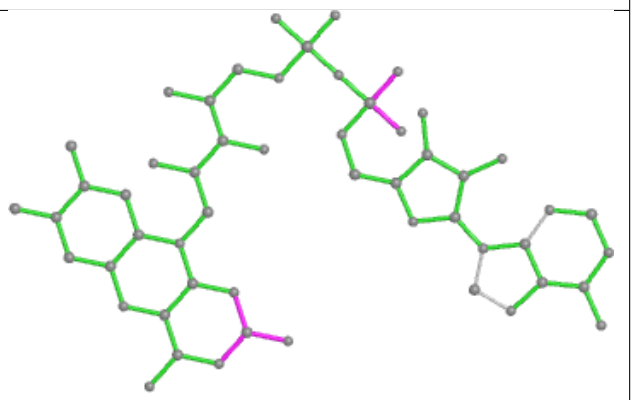


Rings

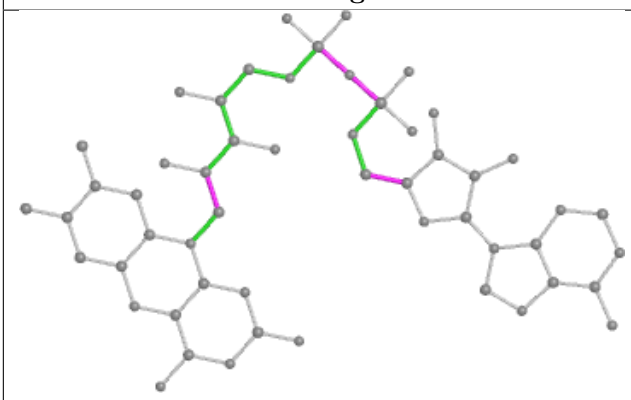
Ligand FAD N 1001



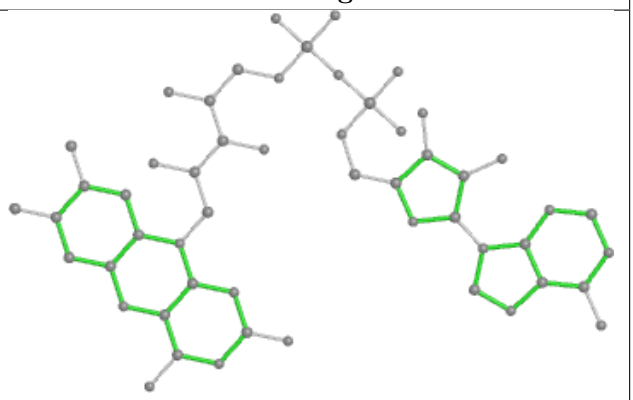
Bond lengths



Bond angles

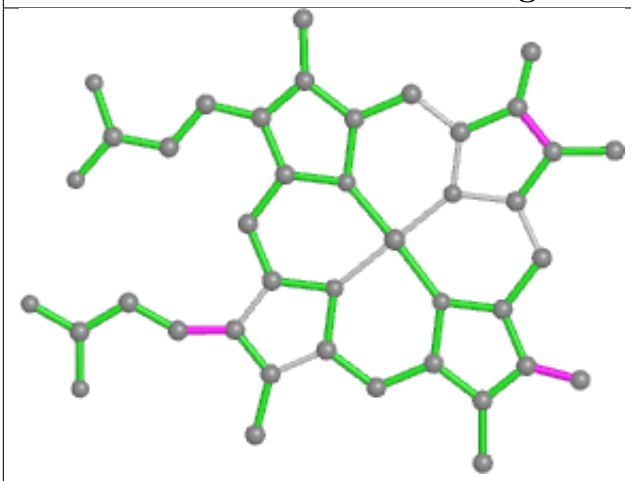


Torsions

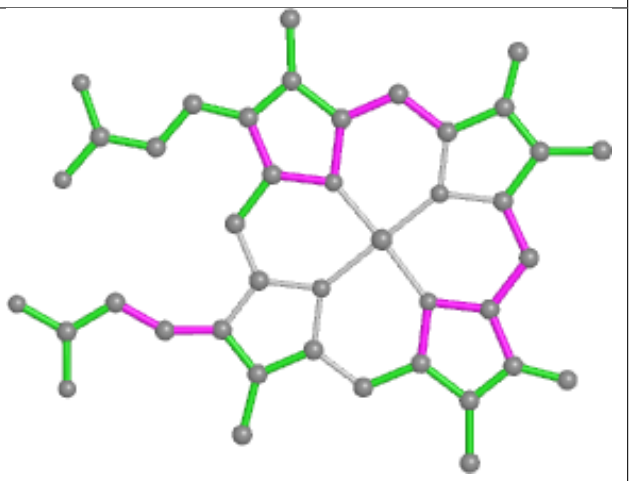


Rings

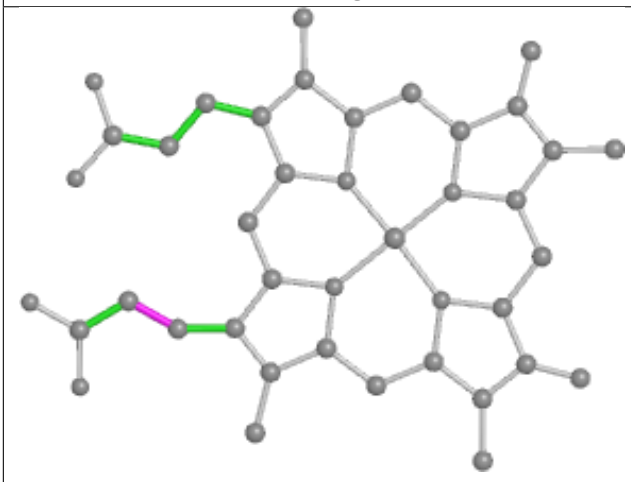
Ligand HEM C 201



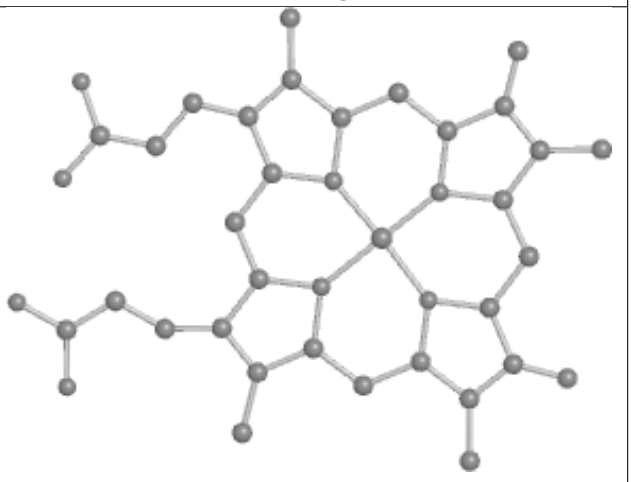
Bond lengths



Bond angles

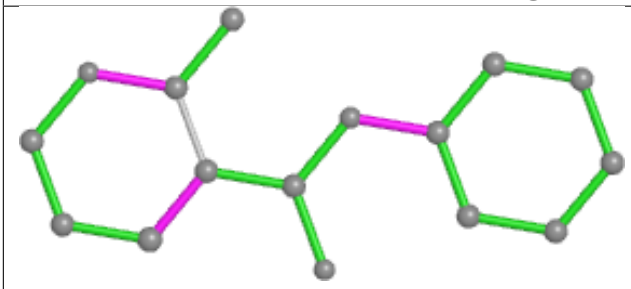


Torsions

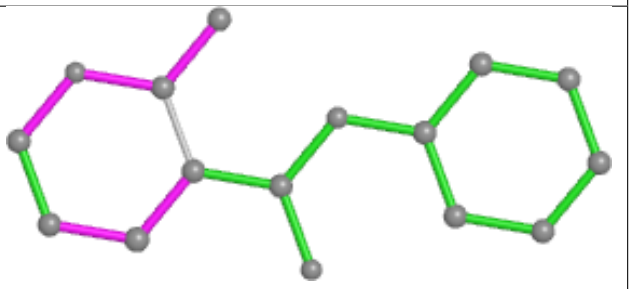


Rings

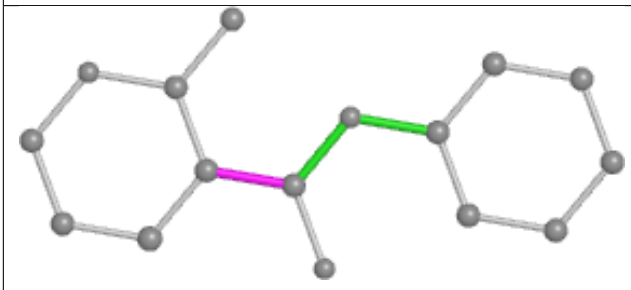
Ligand CBE P 202



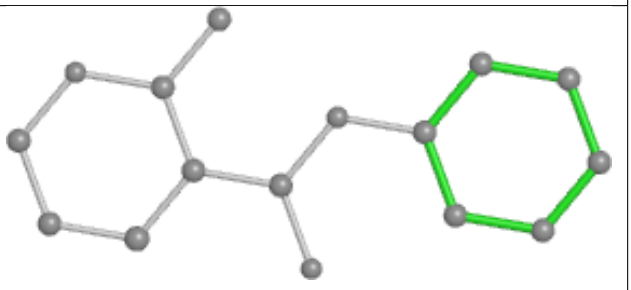
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	612/621 (98%)	-0.21	1 (0%)	95	95	20, 31, 54, 93	4 (0%)
1	N	612/621 (98%)	-0.17	1 (0%)	95	95	19, 31, 54, 96	6 (0%)
2	B	240/252 (95%)	-0.17	2 (0%)	86	87	21, 32, 50, 112	1 (0%)
2	O	241/252 (95%)	-0.13	3 (1%)	79	80	17, 31, 51, 109	0
3	C	139/140 (99%)	0.15	2 (1%)	75	76	30, 45, 80, 88	1 (0%)
3	P	139/140 (99%)	0.25	6 (4%)	35	36	29, 46, 87, 102	0
4	D	101/103 (98%)	0.25	4 (3%)	38	40	34, 53, 78, 86	0
4	Q	101/103 (98%)	0.44	11 (10%)	5	5	36, 55, 78, 93	0
All	All	2185/2232 (97%)	-0.08	30 (1%)	75	76	17, 33, 66, 112	12 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	248	LYS	5.7
4	Q	28	TYR	5.5
1	N	10	THR	5.2
4	Q	93	ILE	4.9
4	Q	103	ILE	4.3

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	UNL	O	1222	1/-	0.04	0.30	73,73,73,73	0
9	UNL	A	1423	1/-	0.41	0.26	64,64,64,64	0
9	UNL	B	1188	1/-	0.44	0.22	48,48,48,48	0
9	UNL	A	1413	1/-	0.49	0.21	49,49,49,49	0
9	UNL	P	253	3/-	0.52	0.45	83,83,85,91	0
9	UNL	N	1433	1/-	0.57	0.15	60,60,60,60	0
9	UNL	B	1211	1/-	0.58	0.19	61,61,61,61	0
9	UNL	A	1378	2/-	0.58	0.36	64,64,64,67	0
9	UNL	Q	218	12/-	0.58	0.46	58,80,96,103	0
9	UNL	D	221	14/-	0.59	0.37	62,91,106,111	0
9	UNL	N	1427	1/-	0.60	0.20	45,45,45,45	0
9	UNL	P	250	6/-	0.61	0.25	69,74,80,82	0
9	UNL	O	1200	3/-	0.61	0.46	81,81,90,92	0
9	UNL	B	1179	4/-	0.61	0.29	63,70,73,73	0
9	UNL	N	1385	4/-	0.62	0.23	72,75,76,82	0
9	UNL	D	227	1/-	0.62	0.25	75,75,75,75	0
9	UNL	N	1406	2/-	0.63	0.32	28,28,28,31	2
9	UNL	O	1215	1/-	0.64	0.16	47,47,47,47	0
9	UNL	C	251[B]	1/-	0.64	0.30	37,37,37,37	1
9	UNL	C	256	1/-	0.64	0.21	47,47,47,47	0
9	UNL	N	1434	1/-	0.64	0.27	58,58,58,58	0
9	UNL	C	251[A]	1/-	0.64	0.30	11,11,11,11	1
9	UNL	A	1377	4/-	0.65	0.34	75,76,79,81	0
9	UNL	N	1428	1/-	0.66	0.34	47,47,47,47	0
9	UNL	P	255	1/-	0.67	0.31	54,54,54,54	0
9	UNL	A	1427	1/-	0.68	0.21	59,59,59,59	0
9	UNL	A	1415	1/-	0.70	0.20	60,60,60,60	0
9	UNL	N	1400	2/-	0.70	0.18	66,66,66,75	0
9	UNL	N	1417[A]	1/-	0.72	0.53	22,22,22,22	1
9	UNL	N	1417[B]	1/-	0.72	0.53	21,21,21,21	1
9	UNL	B	1185	1/-	0.72	0.49	59,59,59,59	0
9	UNL	A	1403	1/-	0.72	0.24	50,50,50,50	0
9	UNL	B	1206	1/-	0.72	0.24	63,63,63,63	0
9	UNL	A	1373	3/-	0.72	0.35	39,39,57,70	0
9	UNL	N	1437	1/-	0.72	0.19	52,52,52,52	0
9	UNL	N	1384	2/-	0.73	0.31	67,67,67,71	0
9	UNL	A	1375	3/-	0.73	0.17	74,74,76,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	UNL	D	220	13/-	0.74	0.31	50,72,97,97	0
9	UNL	N	1388	14/-	0.74	0.49	36,54,70,72	14
9	UNL	B	1180	3/-	0.74	0.19	57,57,66,79	0
9	UNL	P	254	1/-	0.75	0.20	56,56,56,56	0
9	UNL	O	1197	3/-	0.75	0.17	71,71,76,79	0
9	UNL	P	256	1/-	0.75	0.30	57,57,57,57	0
9	UNL	P	257	1/-	0.75	0.12	66,66,66,66	0
9	UNL	Q	213	7/-	0.75	0.58	71,81,89,93	7
9	UNL	Q	216	9/-	0.75	0.26	59,64,75,76	0
9	UNL	N	1397	3/-	0.75	0.19	50,50,56,74	0
17	BOG	P	204	20/20	0.75	0.33	64,83,102,104	0
9	UNL	O	1209[B]	1/-	0.76	0.30	24,24,24,24	1
9	UNL	B	1181	3/-	0.76	0.18	54,54,59,61	0
9	UNL	A	1380	7/-	0.76	0.28	20,52,57,66	7
9	UNL	C	244	3/-	0.76	0.20	45,45,59,60	0
9	UNL	P	252	19/-	0.76	0.92	42,61,85,88	19
9	UNL	A	1418	1/-	0.76	0.10	65,65,65,65	0
9	UNL	O	1209[A]	1/-	0.76	0.30	45,45,45,45	1
9	UNL	A	1394	1/-	0.77	0.20	62,62,62,62	0
9	UNL	B	1177	3/-	0.77	0.22	55,55,64,65	0
9	UNL	O	1196	3/-	0.77	0.20	63,63,73,83	0
9	UNL	O	1214[A]	1/-	0.77	0.30	27,27,27,27	1
9	UNL	O	1214[B]	1/-	0.77	0.30	29,29,29,29	1
9	UNL	A	1408	1/-	0.77	0.13	58,58,58,58	0
9	UNL	A	1421	1/-	0.78	0.25	49,49,49,49	0
9	UNL	B	1212	1/-	0.78	0.14	51,51,51,51	0
9	UNL	N	1410	4/-	0.78	0.35	17,25,27,37	4
9	UNL	B	1171	7/-	0.78	0.24	54,72,78,79	0
9	UNL	A	1372	2/-	0.78	0.23	34,34,34,53	0
9	UNL	D	224	6/-	0.78	0.41	81,86,87,92	0
9	UNL	C	260	1/-	0.79	0.27	55,55,55,55	0
9	UNL	A	1385[B]	1/-	0.79	0.33	21,21,21,21	1
9	UNL	A	1366	3/-	0.79	0.22	47,47,64,65	0
9	UNL	A	1368	4/-	0.79	0.37	33,37,38,40	4
9	UNL	N	1435	1/-	0.79	0.21	56,56,56,56	0
9	UNL	C	255[A]	1/-	0.79	0.20	28,28,28,28	1
9	UNL	Q	215	3/-	0.79	0.16	38,38,61,64	0
9	UNL	N	1446	1/-	0.79	0.22	59,59,59,59	0
9	UNL	C	255[B]	1/-	0.79	0.20	29,29,29,29	1
17	BOG	D	201	17/20	0.79	0.23	61,67,79,82	0
9	UNL	A	1385[A]	1/-	0.79	0.33	45,45,45,45	1
9	UNL	C	245	2/-	0.80	0.18	68,68,68,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	UNL	O	1195	3/-	0.80	0.20	48,48,63,78	0
9	UNL	A	1392	1/-	0.80	0.20	62,62,62,62	0
9	UNL	C	243	9/-	0.80	0.42	54,66,84,84	0
9	UNL	B	1193	1/-	0.80	0.18	53,53,53,53	0
9	UNL	N	1421[A]	1/-	0.80	0.24	33,33,33,33	1
9	UNL	N	1421[B]	1/-	0.80	0.24	24,24,24,24	1
9	UNL	N	1438	1/-	0.80	0.15	58,58,58,58	0
9	UNL	C	257	1/-	0.81	0.19	58,58,58,58	0
8	AZI	B	1005	3/3	0.81	0.21	54,54,65,71	0
9	UNL	A	1367	15/-	0.81	0.23	40,59,71,77	15
9	UNL	C	252[A]	1/-	0.81	0.16	32,32,32,32	1
9	UNL	C	252[B]	1/-	0.81	0.16	34,34,34,34	1
9	UNL	A	1417	1/-	0.81	0.22	60,60,60,60	0
9	UNL	D	229	1/-	0.81	0.18	55,55,55,55	0
9	UNL	A	1376	3/-	0.81	0.15	61,61,66,73	0
9	UNL	O	1221	1/-	0.81	0.23	36,36,36,36	0
9	UNL	O	1192	3/-	0.81	0.14	36,36,49,59	0
9	UNL	O	1224	1/-	0.81	0.35	60,60,60,60	0
9	UNL	B	1208	1/-	0.81	0.19	51,51,51,51	0
9	UNL	N	1401	3/-	0.82	0.15	49,49,57,73	0
9	UNL	A	1412	1/-	0.82	0.15	39,39,39,39	0
9	UNL	N	1407	3/-	0.82	0.32	38,38,45,53	3
9	UNL	B	1205	1/-	0.82	0.23	44,44,44,44	0
9	UNL	O	1193	7/-	0.82	0.42	57,62,66,72	7
9	UNL	N	1426	1/-	0.82	0.14	55,55,55,55	0
9	UNL	B	1190	1/-	0.83	0.15	53,53,53,53	0
9	UNL	O	1202	5/-	0.83	0.35	53,65,68,69	0
9	UNL	O	1223	1/-	0.83	0.76	54,54,54,54	0
9	UNL	N	1390	2/-	0.83	0.17	51,51,51,63	0
9	UNL	O	1226	1/-	0.83	0.12	55,55,55,55	0
9	UNL	B	1187	1/-	0.83	0.25	49,49,49,49	0
9	UNL	Q	217	3/-	0.83	0.13	52,52,64,64	0
9	UNL	B	1209	1/-	0.83	0.13	52,52,52,52	0
9	UNL	B	1172	4/-	0.83	0.18	68,71,74,77	0
9	UNL	N	1444	1/-	0.83	0.14	59,59,59,59	0
9	UNL	A	1396[B]	1/-	0.84	0.17	36,36,36,36	1
9	UNL	O	1204	3/-	0.84	0.16	54,54,55,66	0
9	UNL	N	1415[A]	1/-	0.84	0.20	16,16,16,16	1
9	UNL	N	1415[B]	1/-	0.84	0.20	22,22,22,22	1
9	UNL	A	1397[A]	1/-	0.84	0.26	25,25,25,25	1
9	UNL	A	1397[B]	1/-	0.84	0.26	18,18,18,18	1
9	UNL	B	1200	1/-	0.84	0.18	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	UNL	B	1204	1/-	0.84	0.44	20,20,20,20	1
9	UNL	D	226[A]	1/-	0.84	0.38	47,47,47,47	1
9	UNL	D	226[B]	1/-	0.84	0.38	15,15,15,15	1
9	UNL	B	1173	3/-	0.84	0.14	42,42,47,64	0
9	UNL	N	1432	1/-	0.84	0.21	51,51,51,51	0
9	UNL	A	1396[A]	1/-	0.84	0.17	20,20,20,20	1
9	UNL	N	1412[A]	1/-	0.85	0.20	21,21,21,21	1
9	UNL	N	1412[B]	1/-	0.85	0.20	35,35,35,35	1
9	UNL	C	248[A]	1/-	0.85	0.25	28,28,28,28	1
9	UNL	C	248[B]	1/-	0.85	0.25	31,31,31,31	1
9	UNL	A	1422	1/-	0.85	0.15	54,54,54,54	0
9	UNL	O	1206[A]	1/-	0.85	0.24	33,33,33,33	1
9	UNL	O	1206[B]	1/-	0.85	0.24	17,17,17,17	1
9	UNL	D	223	4/-	0.85	0.44	60,60,67,74	0
9	UNL	N	1402	3/-	0.85	0.21	24,24,31,41	3
9	UNL	O	1211[A]	1/-	0.85	0.21	33,33,33,33	1
9	UNL	O	1211[B]	1/-	0.85	0.21	8,8,8,8	1
9	UNL	Q	214[A]	17/-	0.85	0.38	20,42,49,49	17
9	UNL	Q	214[B]	16/-	0.85	0.38	37,46,55,58	16
9	UNL	N	1445	1/-	0.85	0.13	50,50,50,50	0
9	UNL	B	1189	1/-	0.85	0.32	47,47,47,47	0
9	UNL	A	1387	1/-	0.85	0.41	47,47,47,47	0
9	UNL	O	1218	1/-	0.85	0.32	56,56,56,56	0
9	UNL	N	1408	4/-	0.85	0.14	57,59,60,67	0
9	UNL	N	1389	2/-	0.85	0.11	63,63,63,73	0
18	UMQ	P	203	26/34	0.85	0.21	42,58,107,113	0
9	UNL	B	1174	3/-	0.86	0.19	62,62,63,74	0
9	UNL	A	1398[B]	1/-	0.86	0.18	21,21,21,21	1
9	UNL	A	1425	1/-	0.86	0.13	53,53,53,53	0
9	UNL	O	1213[A]	1/-	0.86	0.18	22,22,22,22	1
9	UNL	O	1213[B]	1/-	0.86	0.18	21,21,21,21	1
9	UNL	B	1194	1/-	0.86	0.17	52,52,52,52	0
9	UNL	A	1384	2/-	0.86	0.12	55,55,55,63	0
9	UNL	B	1201[A]	1/-	0.86	0.29	17,17,17,17	1
9	UNL	O	1198	4/-	0.86	0.14	52,60,61,70	0
9	UNL	B	1201[B]	1/-	0.86	0.29	42,42,42,42	1
9	UNL	A	1428	1/-	0.86	0.13	69,69,69,69	0
9	UNL	N	1395	6/-	0.86	0.19	51,57,61,70	6
9	UNL	A	1419	1/-	0.86	0.16	60,60,60,60	0
9	UNL	A	1398[A]	1/-	0.86	0.18	31,31,31,31	1
9	UNL	P	249	9/-	0.86	0.48	58,72,86,93	0
9	UNL	A	1416	1/-	0.86	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	UNL	A	1399[A]	1/-	0.87	0.22	24,24,24,24	1
9	UNL	D	222	9/-	0.87	0.16	52,61,65,66	0
9	UNL	A	1399[B]	1/-	0.87	0.22	29,29,29,29	1
9	UNL	O	1199	5/-	0.87	0.14	37,46,55,64	0
9	UNL	Q	219	5/-	0.87	0.18	47,50,74,79	0
17	BOG	C	203	18/20	0.87	0.33	56,77,95,104	0
9	UNL	N	1391	3/-	0.87	0.12	46,46,59,59	0
9	UNL	A	1383	5/-	0.87	0.43	65,66,72,73	0
9	UNL	B	1176	4/-	0.87	0.13	68,70,76,76	4
9	UNL	O	1216[B]	1/-	0.88	0.25	35,35,35,35	1
9	UNL	N	1404	7/-	0.88	0.22	37,62,71,71	0
9	UNL	N	1424	1/-	0.88	0.21	47,47,47,47	0
9	UNL	B	1184[A]	1/-	0.88	0.30	22,22,22,22	1
9	UNL	B	1184[B]	1/-	0.88	0.30	36,36,36,36	1
9	UNL	A	1381	3/-	0.88	0.14	31,31,55,67	0
9	UNL	A	1379	3/-	0.88	0.26	21,21,42,58	3
9	UNL	N	1393	3/-	0.88	0.12	64,64,69,73	0
9	UNL	O	1216[A]	1/-	0.88	0.25	44,44,44,44	1
9	UNL	N	1399	1/-	0.89	0.17	40,40,40,40	0
9	UNL	O	1227	1/-	0.89	0.11	67,67,67,67	0
9	UNL	A	1370	4/-	0.89	0.14	40,45,55,91	0
9	UNL	A	1395	1/-	0.89	0.19	44,44,44,44	0
9	UNL	A	1400[A]	1/-	0.89	0.22	26,26,26,26	1
9	UNL	N	1429	1/-	0.89	0.19	54,54,54,54	0
9	UNL	A	1400[B]	1/-	0.89	0.22	24,24,24,24	1
9	UNL	N	1383	2/-	0.89	0.20	56,56,56,58	0
9	UNL	A	1391	1/-	0.89	0.22	60,60,60,60	0
9	UNL	B	1196	1/-	0.89	0.46	46,46,46,46	0
9	UNL	B	1197	1/-	0.89	0.17	46,46,46,46	0
9	UNL	N	1411	2/-	0.89	0.15	55,55,55,57	0
9	UNL	A	1429	1/-	0.89	0.12	66,66,66,66	0
9	UNL	A	1431	1/-	0.89	0.14	47,47,47,47	0
9	UNL	A	1405	1/-	0.89	0.15	44,44,44,44	0
9	UNL	N	1392	2/-	0.89	0.27	55,55,55,61	0
9	UNL	A	1406	1/-	0.89	0.23	47,47,47,47	0
9	UNL	A	1386	1/-	0.89	0.10	42,42,42,42	0
14	GOL	N	1005	6/6	0.89	0.21	35,36,38,49	6
9	UNL	N	1419[A]	1/-	0.89	0.22	0,0,0,0	1
9	UNL	N	1419[B]	1/-	0.89	0.22	41,41,41,41	1
9	UNL	N	1396	3/-	0.89	0.12	27,27,41,50	0
9	UNL	D	225	1/-	0.89	0.37	48,48,48,48	0
9	UNL	N	1416[A]	1/-	0.90	0.22	24,24,24,24	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	UNL	N	1416[B]	1/-	0.90	0.22	34,34,34,34	1
9	UNL	B	1199	1/-	0.90	0.17	45,45,45,45	0
9	UNL	A	1409	1/-	0.90	0.30	44,44,44,44	0
9	UNL	D	228	1/-	0.90	0.13	59,59,59,59	0
8	AZI	A	1004	3/3	0.90	0.11	41,41,47,59	0
9	UNL	A	1374	2/-	0.90	0.19	54,54,54,63	2
9	UNL	N	1440	1/-	0.90	0.16	57,57,57,57	0
9	UNL	N	1441	1/-	0.90	0.16	52,52,52,52	0
9	UNL	N	1443	1/-	0.90	0.11	51,51,51,51	0
9	UNL	B	1213	1/-	0.90	0.15	42,42,42,42	0
9	UNL	B	1195	1/-	0.90	0.09	45,45,45,45	0
9	UNL	Q	221	1/-	0.90	0.10	51,51,51,51	0
9	UNL	A	1430	1/-	0.90	0.26	51,51,51,51	0
9	UNL	A	1369	4/-	0.90	0.13	41,45,46,53	0
9	UNL	O	1212[A]	1/-	0.90	0.30	41,41,41,41	1
9	UNL	O	1212[B]	1/-	0.90	0.30	33,33,33,33	1
9	UNL	C	246	3/-	0.90	0.16	52,52,58,66	0
9	UNL	N	1405	3/-	0.91	0.12	42,42,57,59	0
9	UNL	A	1401[A]	1/-	0.91	0.22	29,29,29,29	1
9	UNL	B	1207	1/-	0.91	0.22	41,41,41,41	0
9	UNL	A	1401[B]	1/-	0.91	0.22	4,4,4,4	1
9	UNL	N	1409	4/-	0.91	0.12	70,70,73,77	0
9	UNL	B	1191	1/-	0.91	0.27	51,51,51,51	0
9	UNL	N	1422[A]	1/-	0.91	0.23	25,25,25,25	1
9	UNL	N	1422[B]	1/-	0.91	0.23	28,28,28,28	1
9	UNL	B	1210	1/-	0.91	0.49	48,48,48,48	0
9	UNL	C	250[A]	1/-	0.91	0.19	23,23,23,23	1
9	UNL	Q	220	1/-	0.91	0.28	60,60,60,60	0
9	UNL	C	250[B]	1/-	0.91	0.19	24,24,24,24	1
9	UNL	A	1414	1/-	0.91	0.12	47,47,47,47	0
9	UNL	B	1178	3/-	0.91	0.10	54,54,55,59	0
9	UNL	N	1430	1/-	0.91	0.11	41,41,41,41	0
9	UNL	A	1371	2/-	0.91	0.16	35,35,35,43	0
9	UNL	A	1404	1/-	0.91	0.15	57,57,57,57	0
9	UNL	N	1425	1/-	0.92	0.17	30,30,30,30	0
9	UNL	C	249[B]	1/-	0.92	0.23	19,19,19,19	1
9	UNL	N	1418[A]	1/-	0.92	0.16	28,28,28,28	1
9	UNL	O	1225	1/-	0.92	0.11	42,42,42,42	0
9	UNL	N	1418[B]	1/-	0.92	0.16	33,33,33,33	1
9	UNL	N	1387	3/-	0.92	0.12	47,47,56,59	0
9	UNL	O	1203	4/-	0.92	0.20	46,47,49,53	4
9	UNL	B	1202	1/-	0.92	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	UNL	P	251	2/-	0.92	0.39	59,59,59,70	0
9	UNL	B	1203	1/-	0.92	0.37	44,44,44,44	0
9	UNL	N	1398	2/-	0.92	0.19	53,53,53,57	0
9	UNL	C	259	1/-	0.92	0.55	60,60,60,60	0
9	UNL	O	1217	1/-	0.92	0.28	42,42,42,42	0
9	UNL	C	254	1/-	0.92	0.12	33,33,33,33	0
9	UNL	C	249[A]	1/-	0.92	0.23	27,27,27,27	1
9	UNL	B	1182[A]	1/-	0.93	0.24	21,21,21,21	1
9	UNL	B	1182[B]	1/-	0.93	0.24	4,4,4,4	1
9	UNL	N	1394	2/-	0.93	0.12	58,58,58,73	0
9	UNL	N	1431	1/-	0.93	0.16	45,45,45,45	0
9	UNL	A	1424	1/-	0.93	0.11	58,58,58,58	0
9	UNL	A	1402[A]	1/-	0.93	0.18	14,14,14,14	1
9	UNL	A	1426	1/-	0.93	0.15	55,55,55,55	0
9	UNL	A	1402[B]	1/-	0.93	0.18	12,12,12,12	1
9	UNL	A	1411	1/-	0.93	0.16	52,52,52,52	0
9	UNL	A	1382	3/-	0.93	0.15	26,26,31,50	3
9	UNL	N	1423	1/-	0.93	0.16	42,42,42,42	0
9	UNL	A	1393	1/-	0.93	0.20	55,55,55,55	0
9	UNL	A	1390	1/-	0.93	0.61	37,37,37,37	0
9	UNL	B	1192	1/-	0.93	0.13	53,53,53,53	0
8	AZI	N	1004	3/3	0.93	0.15	40,40,48,59	0
9	UNL	N	1420[A]	1/-	0.94	0.35	26,26,26,26	1
9	UNL	N	1420[B]	1/-	0.94	0.35	8,8,8,8	1
9	UNL	B	1183[A]	1/-	0.94	0.23	24,24,24,24	1
9	UNL	B	1198	1/-	0.94	0.26	50,50,50,50	0
9	UNL	B	1183[B]	1/-	0.94	0.23	6,6,6,6	1
9	UNL	O	1201	3/-	0.94	0.11	54,54,67,71	0
9	UNL	N	1403	3/-	0.94	0.17	15,15,21,33	3
9	UNL	B	1175	3/-	0.94	0.21	53,53,65,66	0
9	UNL	C	247	1/-	0.94	0.23	48,48,48,48	0
9	UNL	O	1205	1/-	0.94	0.16	49,49,49,49	0
9	UNL	A	1420	1/-	0.94	0.33	50,50,50,50	0
9	UNL	O	1194	6/-	0.94	0.16	35,43,53,56	0
9	UNL	O	1207[A]	1/-	0.94	0.17	13,13,13,13	1
9	UNL	O	1207[B]	1/-	0.94	0.17	30,30,30,30	1
9	UNL	A	1407	1/-	0.94	0.11	35,35,35,35	0
9	UNL	N	1439	1/-	0.95	0.14	17,17,17,17	1
9	UNL	A	1410	1/-	0.95	0.12	57,57,57,57	0
9	UNL	O	1208[A]	1/-	0.95	0.28	19,19,19,19	1
9	UNL	O	1208[B]	1/-	0.95	0.28	20,20,20,20	1
9	UNL	C	261	1/-	0.95	0.12	55,55,55,55	0

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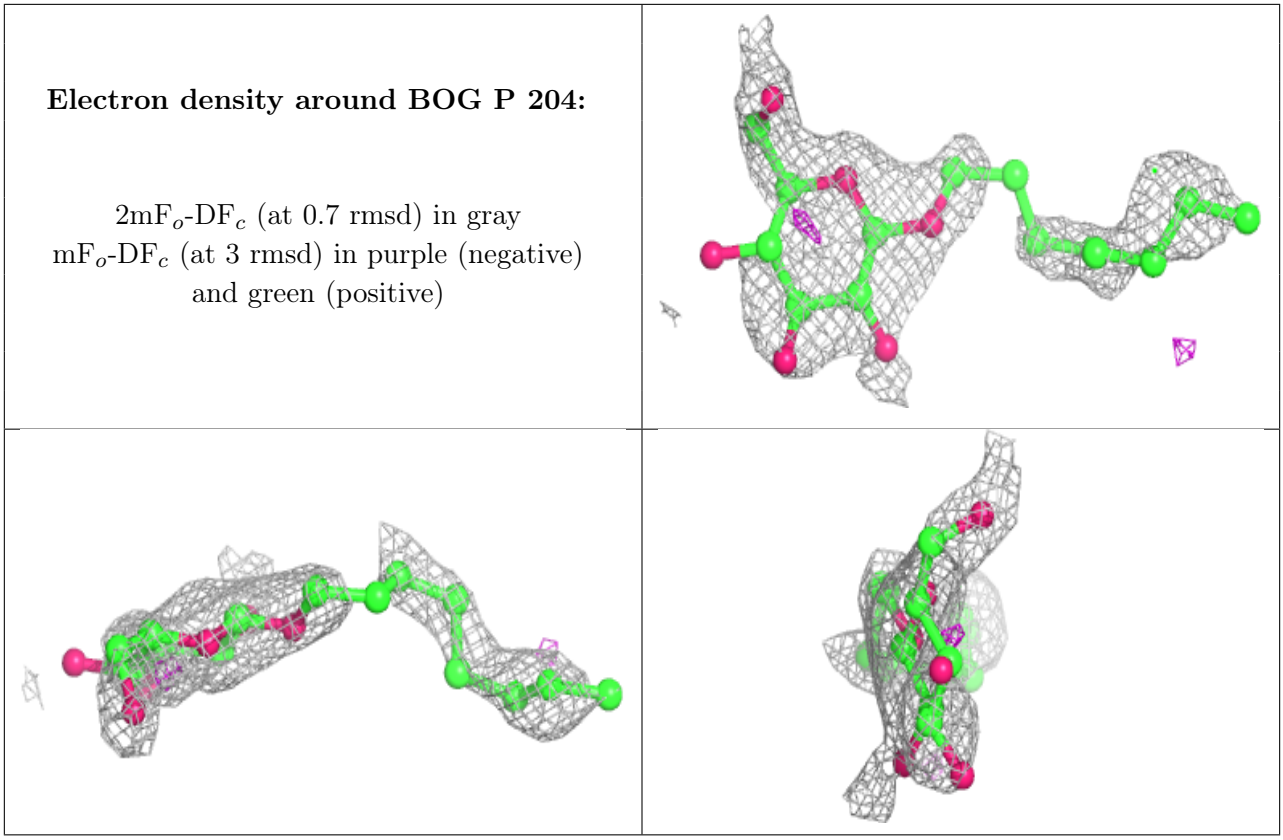
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	GOL	B	1006	6/6	0.95	0.13	32,40,43,45	0
9	UNL	N	1442	1/-	0.95	0.20	51,51,51,51	0
9	UNL	C	258	1/-	0.95	0.20	49,49,49,49	0
9	UNL	N	1413[A]	1/-	0.95	0.27	16,16,16,16	1
9	UNL	N	1413[B]	1/-	0.95	0.27	23,23,23,23	1
9	UNL	C	253	1/-	0.95	0.12	28,28,28,28	1
9	UNL	B	1186[A]	1/-	0.96	0.17	12,12,12,12	1
9	UNL	N	1386	2/-	0.96	0.16	23,23,23,43	2
9	UNL	O	1219	1/-	0.96	0.17	26,26,26,26	1
9	UNL	O	1220	1/-	0.96	0.18	56,56,56,56	0
9	UNL	O	1210	1/-	0.96	0.17	50,50,50,50	0
16	CBE	C	202	16/16	0.96	0.16	29,36,43,47	0
9	UNL	B	1186[B]	1/-	0.96	0.17	4,4,4,4	1
9	UNL	A	1388	1/-	0.96	0.13	35,35,35,35	0
6	Y3P	N	1002	9/9	0.96	0.13	24,29,41,41	0
9	UNL	N	1436	1/-	0.96	0.12	24,24,24,24	0
15	HEM	P	201	41/43	0.97	0.13	28,41,57,63	0
9	UNL	A	1389	1/-	0.97	0.54	45,45,45,45	0
16	CBE	P	202	16/16	0.97	0.12	27,35,47,48	0
5	FAD	A	1001	53/53	0.97	0.12	9,22,32,37	0
9	UNL	N	1414[A]	1/-	0.97	0.17	14,14,14,14	1
9	UNL	N	1414[B]	1/-	0.97	0.17	0,0,0,0	1
6	Y3P	A	1002	9/9	0.97	0.13	22,31,41,50	0
15	HEM	C	201	41/43	0.98	0.12	20,40,55,69	0
5	FAD	N	1001	53/53	0.98	0.12	10,21,29,34	0
7	K	N	1003	1/1	0.99	0.09	28,28,28,28	0
10	FES	B	1001	4/4	0.99	0.14	24,24,24,27	0
10	FES	O	1001	4/4	0.99	0.13	23,25,26,28	0
11	SF4	B	1002	8/8	0.99	0.11	24,26,28,30	0
11	SF4	O	1002	8/8	0.99	0.13	22,27,31,31	0
12	F3S	B	1003	7/7	0.99	0.14	27,28,30,34	0
12	F3S	O	1003	7/7	0.99	0.15	25,28,32,32	0
13	NA	B	1004	1/1	0.99	0.10	25,25,25,25	0
7	K	A	1003	1/1	0.99	0.09	33,33,33,33	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.

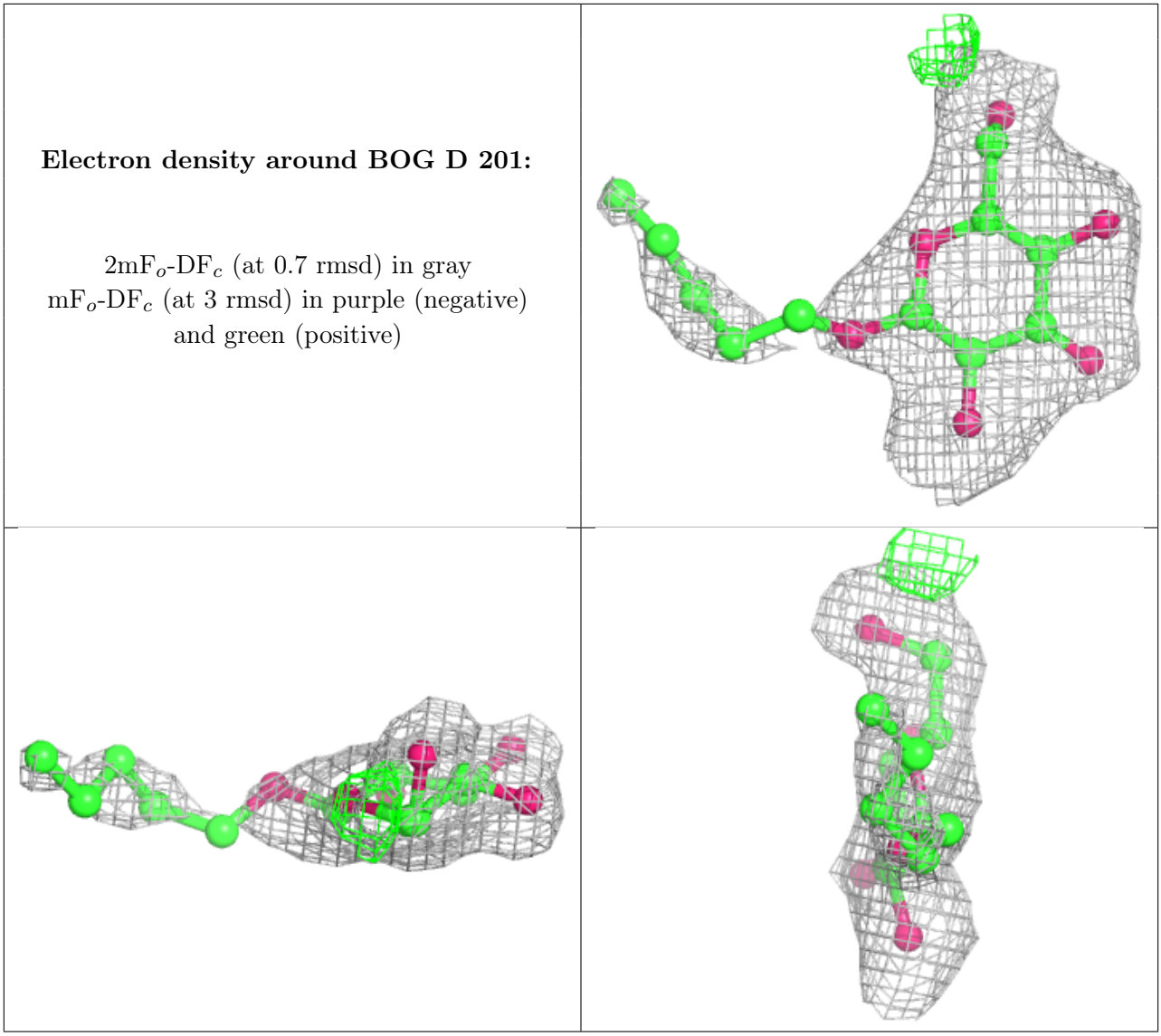
Electron density around BOG P 204:

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



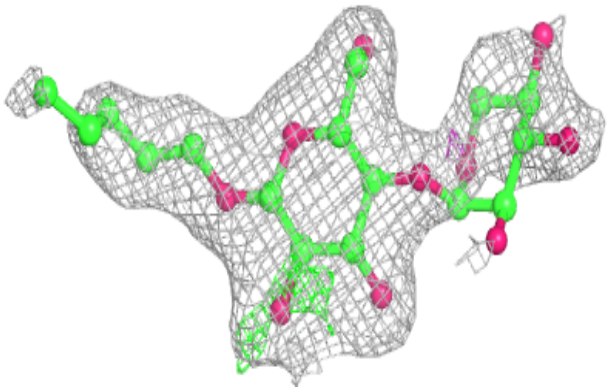
Electron density around BOG D 201:

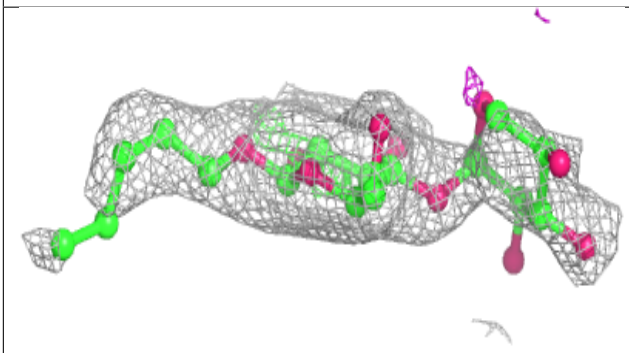
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

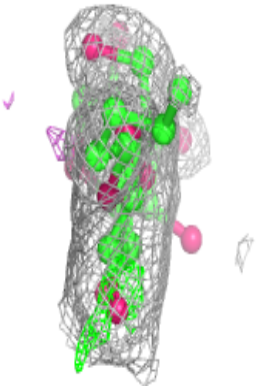


Electron density around UMQ P 203:

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

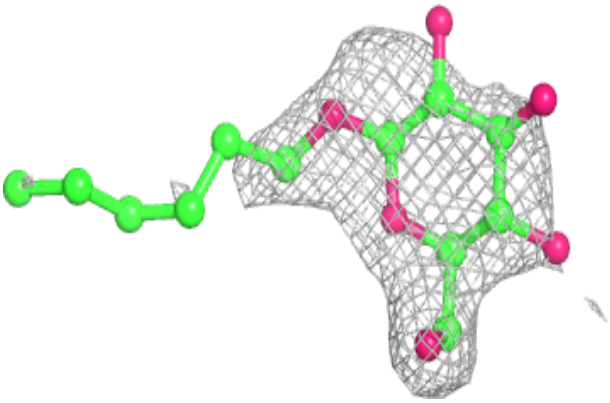


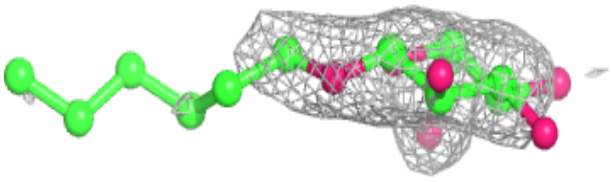


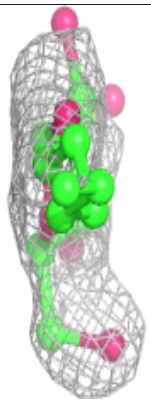


Electron density around BOG C 203:

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

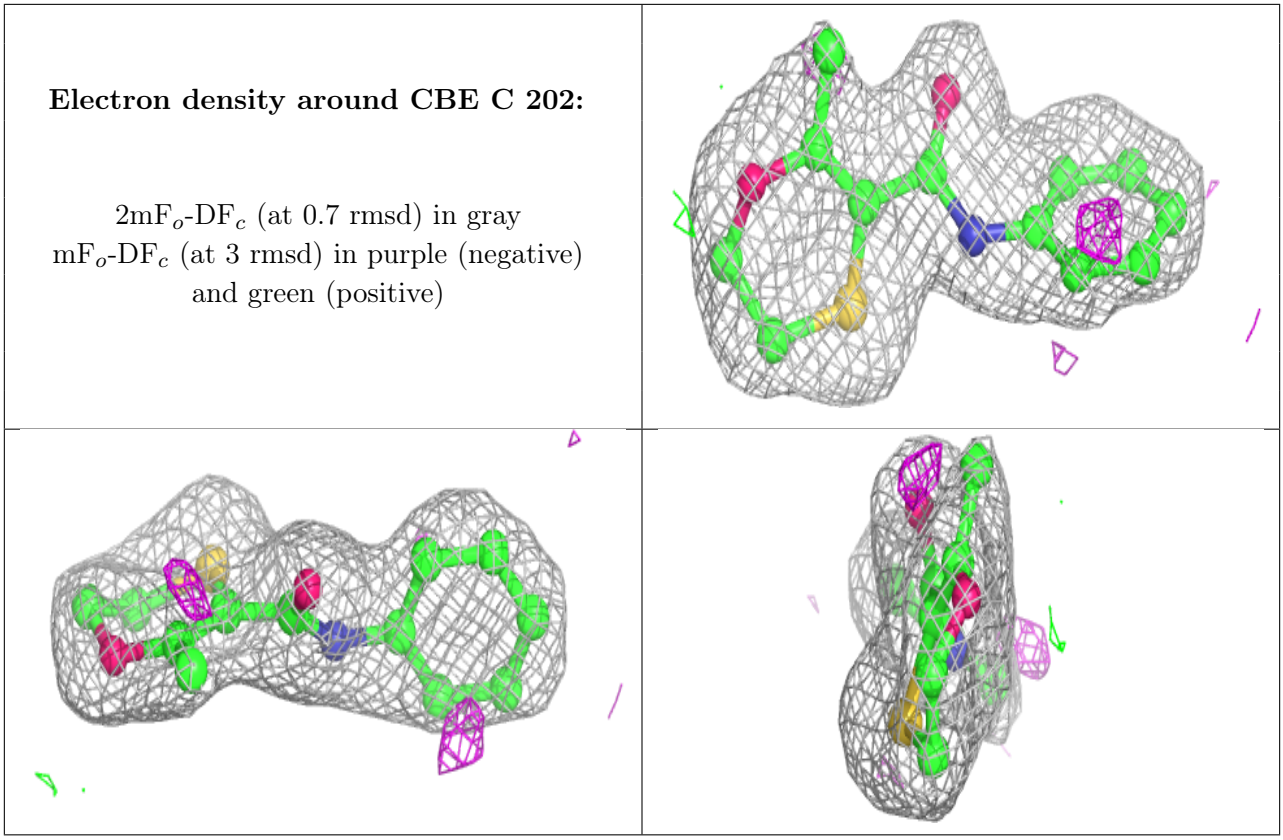






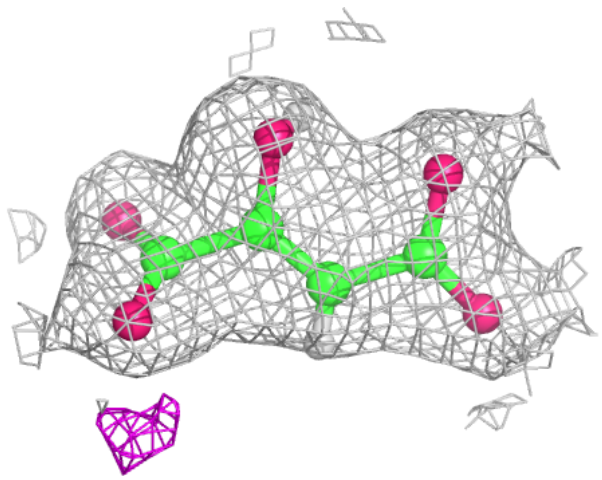
Electron density around CBE C 202:

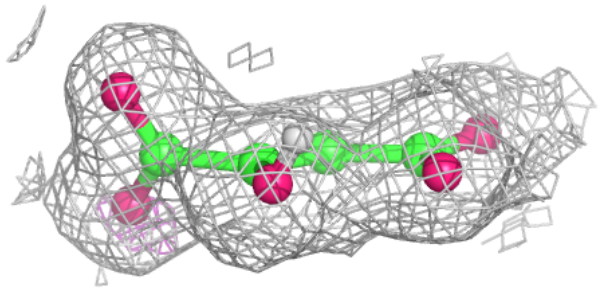
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

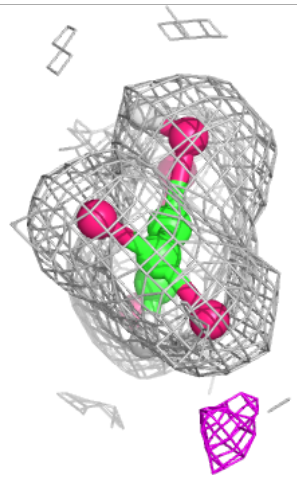


Electron density around Y3P N 1002:

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

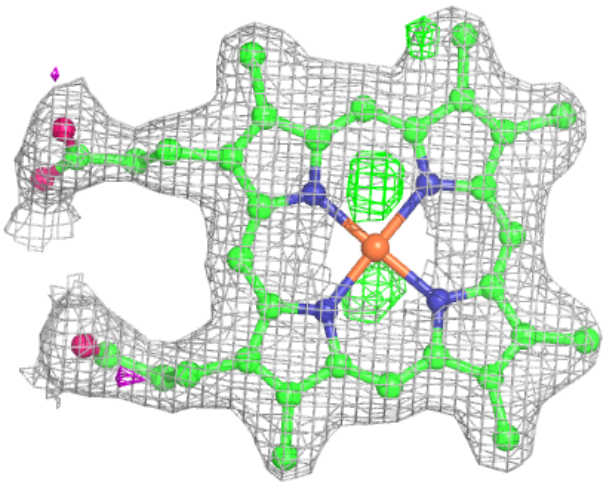


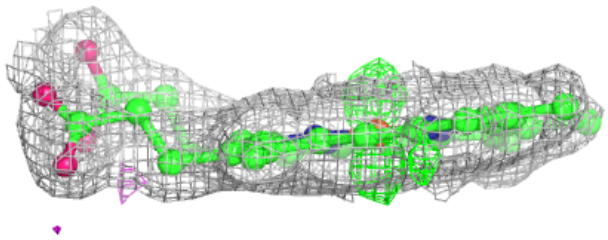


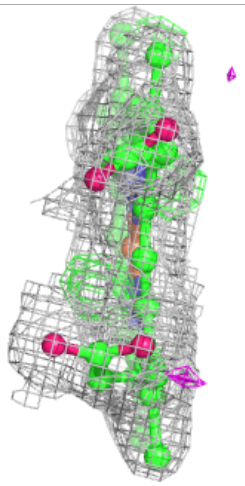


Electron density around HEM P 201:

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

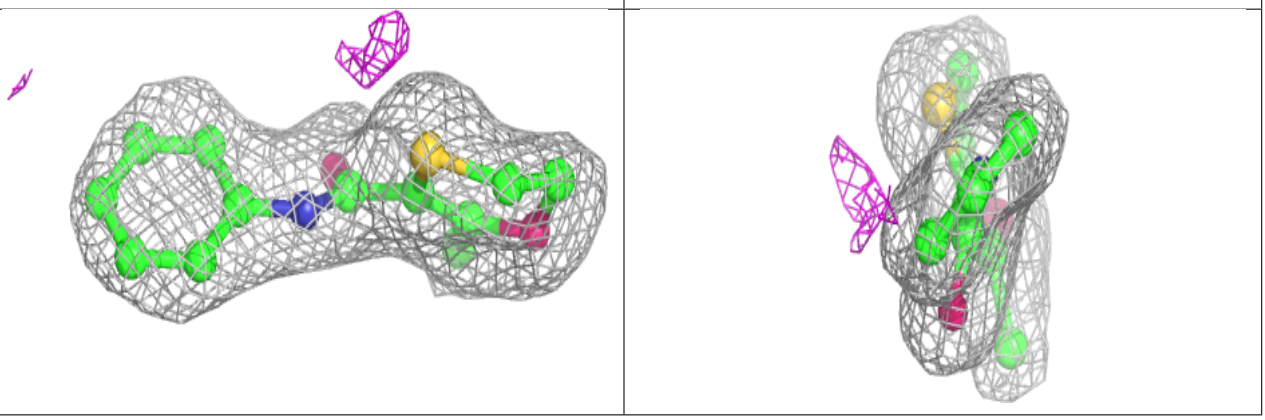






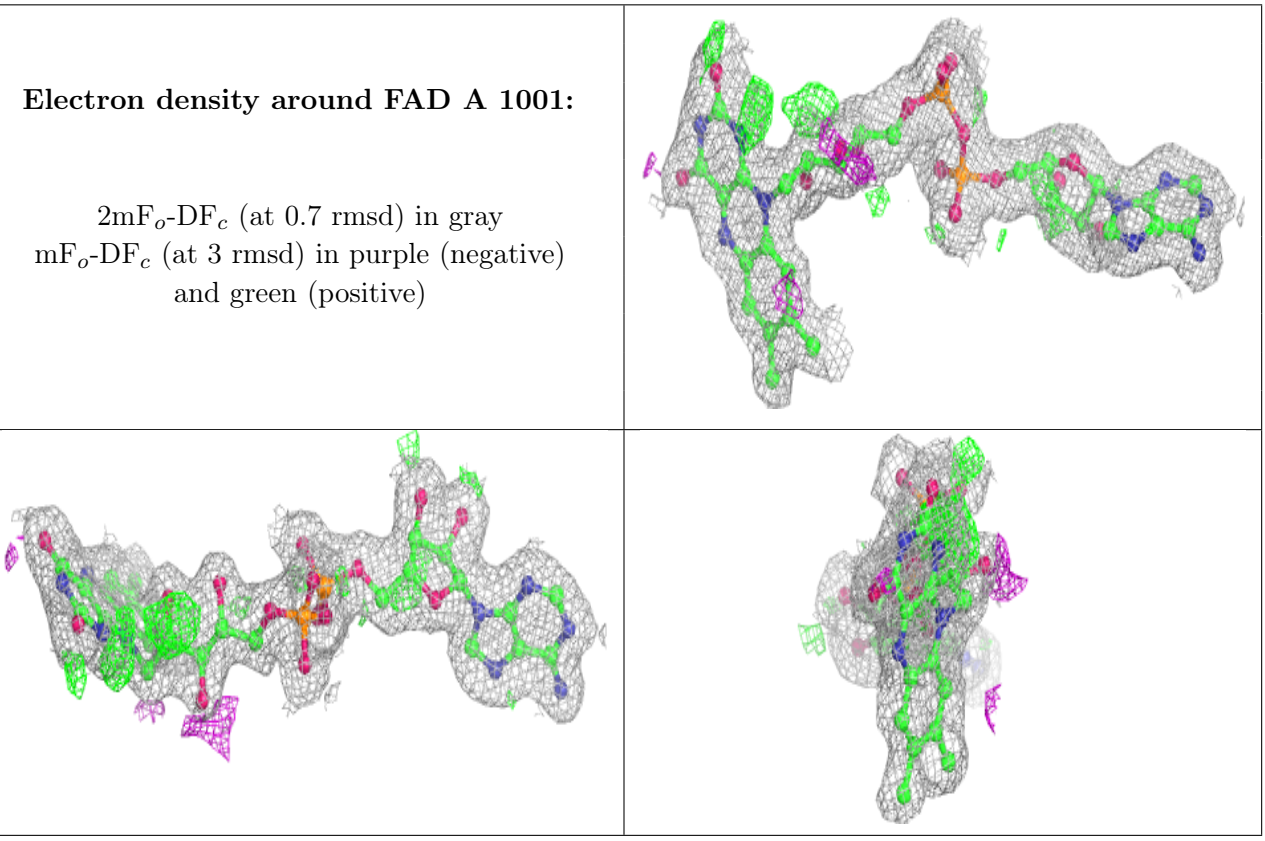
Electron density around CBE P 202:

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



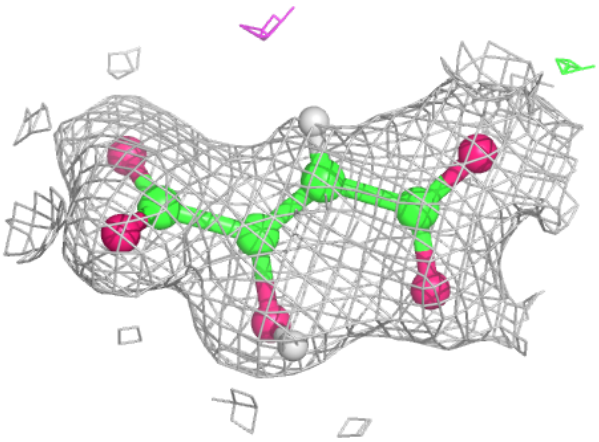
Electron density around FAD A 1001:

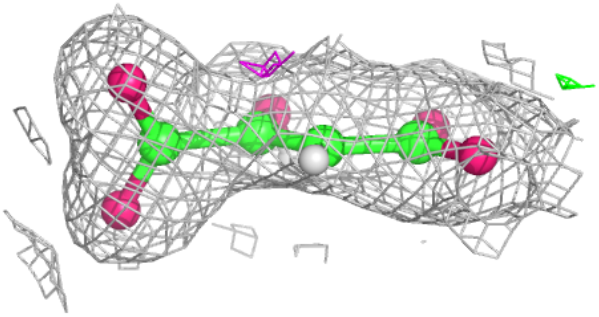
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

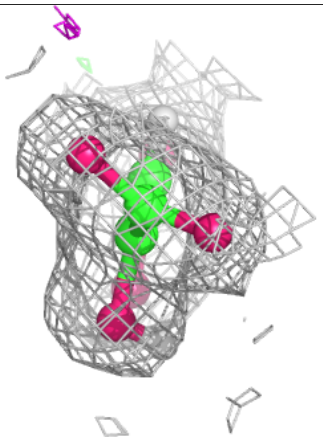


Electron density around Y3P A 1002:

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

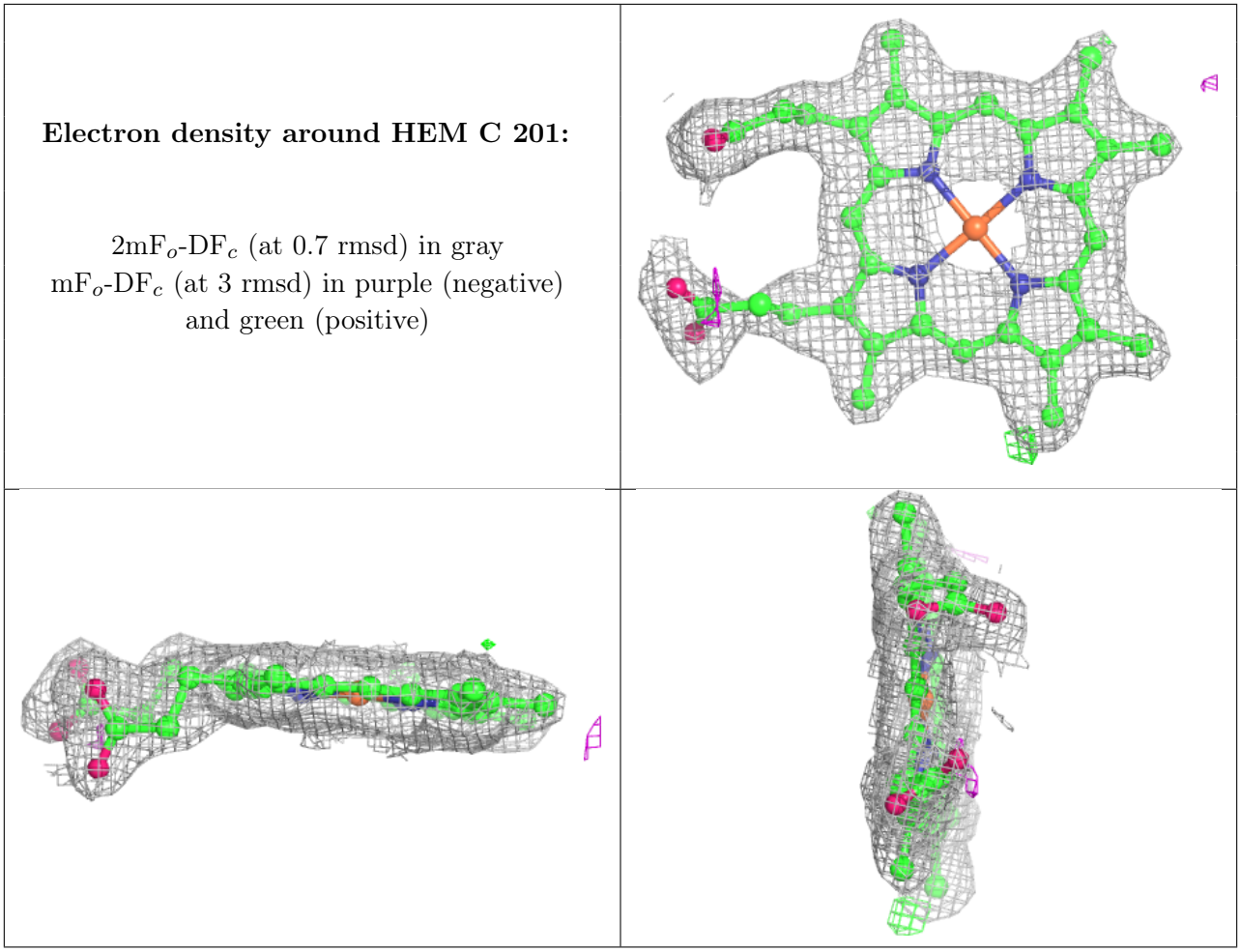






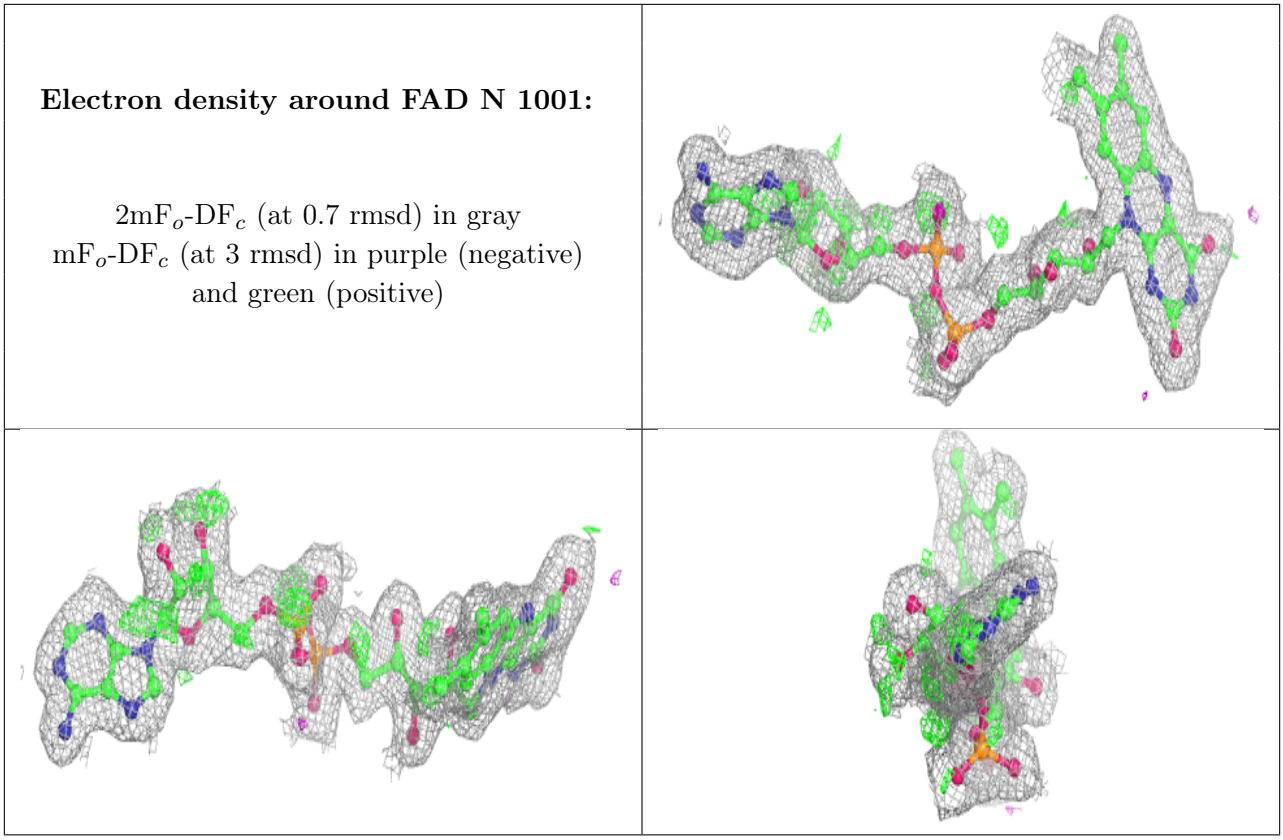
Electron density around HEM C 201:

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



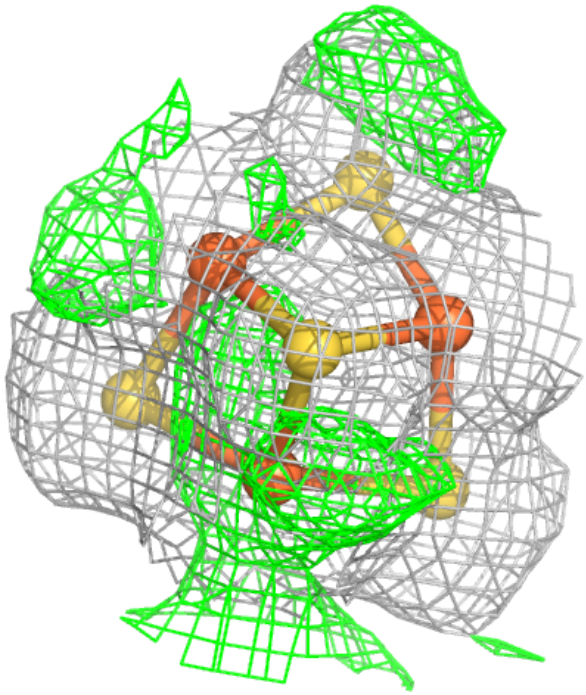
Electron density around FAD N 1001:

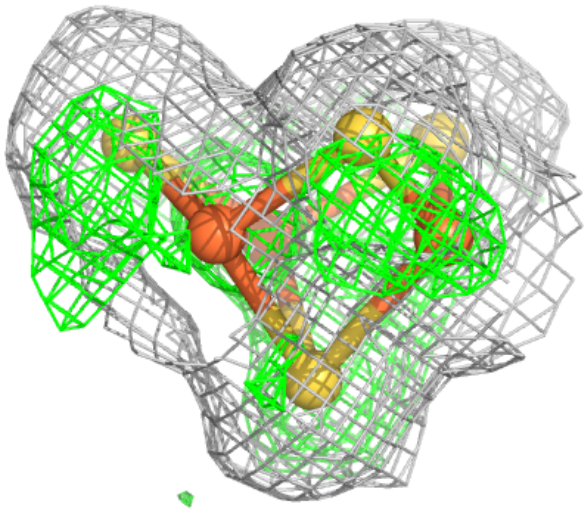
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

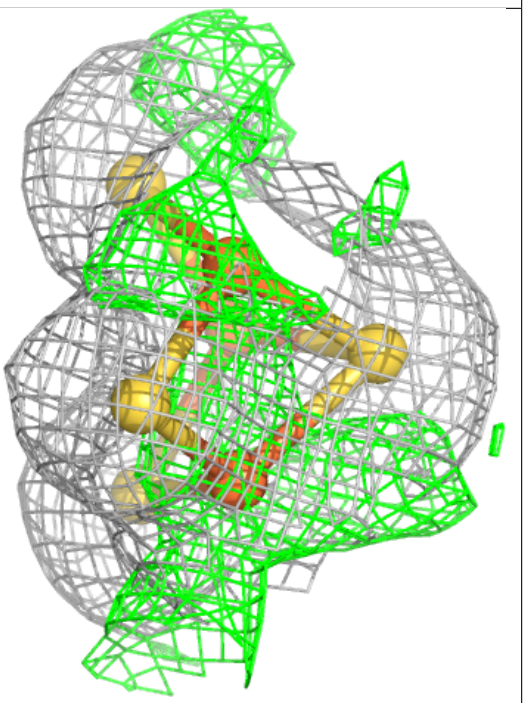


Electron density around F3S B 1003:

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

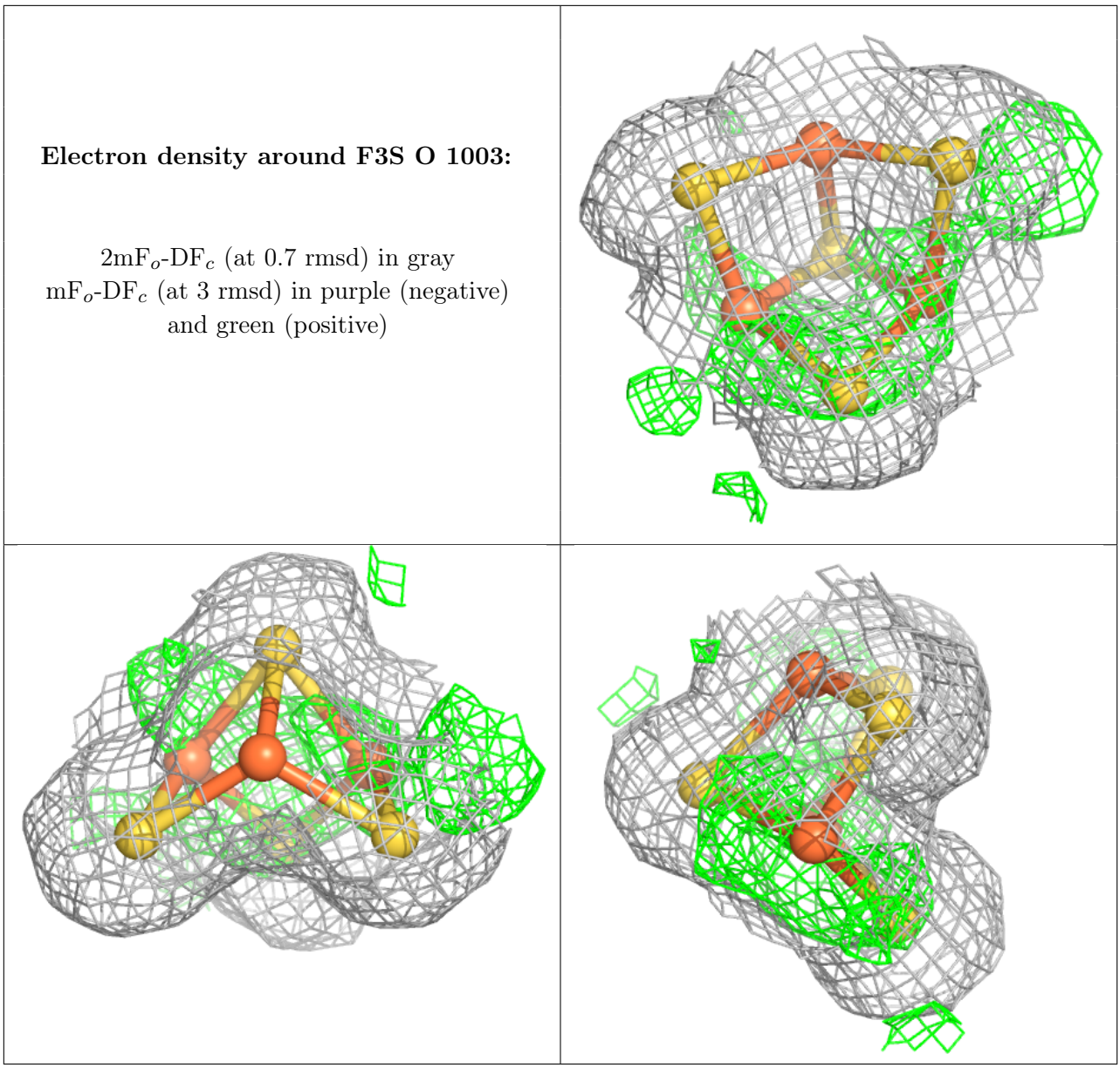






Electron density around F3S O 1003:

$2mF_o$-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.