Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 03:14 AM EDT

PDB ID	:	6MYQ
Title	:	Avian mitochondrial complex II with ferulenol bound
Authors	:	Berry, E.A.; Huang, L.-S.
Deposited on	:	2018-11-02
Resolution	:	1.97 Å(reported)

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

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

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

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

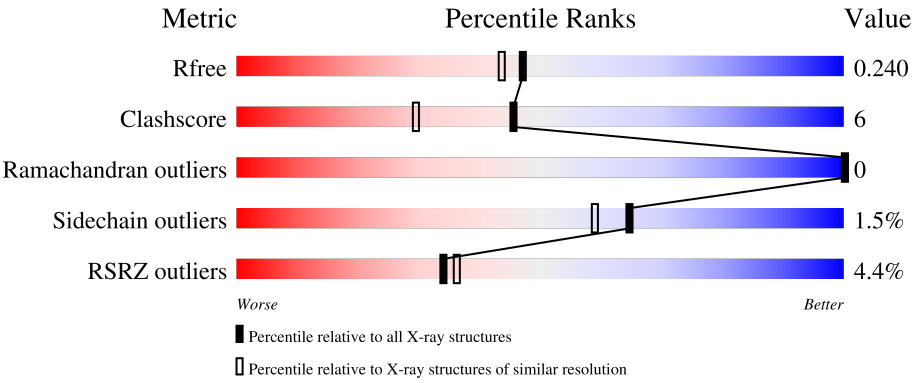
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	3% 83% 15% ·
2	B	252	5% 81% 13% 5%
3	C	140	7% 87% 12% ·
4	D	103	5% 84% 14% ··

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
10	MOH	A	1011	-	-	-	X
6	Y3P	A	1002	-	X	X	-
8	UNL	A	1027	-	-	-	X
8	UNL	C	1021	-	-	-	X
8	UNL	D	203	-	-	X	-
8	UNL	D	207	-	-	-	X
8	UNL	D	212	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 9426 atoms, of which 2 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
			Total	C	N	O	S			
1	A	611	4723	2956	843	895	29	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	239	1921	1215	325	359	22	0	0	0

- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b, large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	139	1076	707	178	186	5	0	0	0

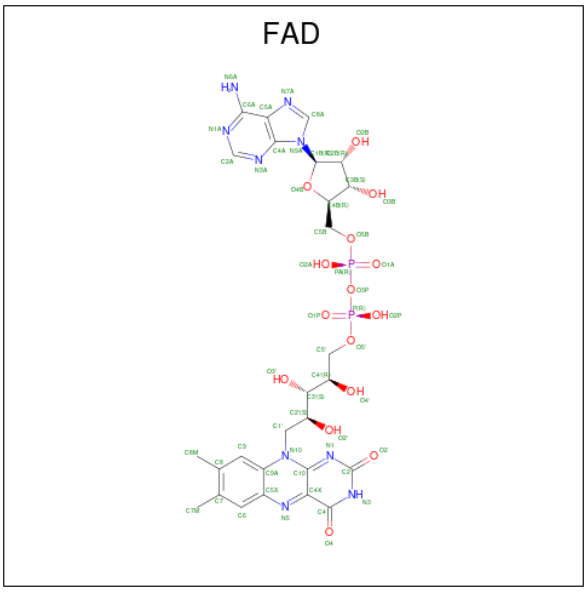
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	139	ALA	SER	conflict	UNP D0VWW3
C	140	MET	GLU	conflict	UNP D0VWW3

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

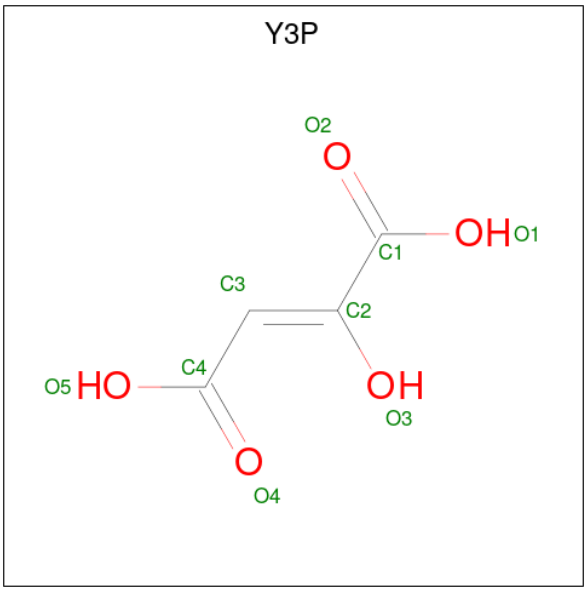
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	102	771	508	122	138	3	0	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	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	0	0
			11	4	2	5		

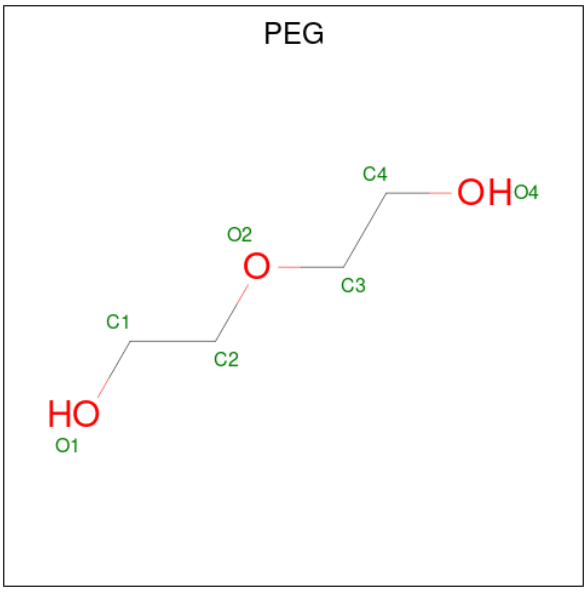
- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 8 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

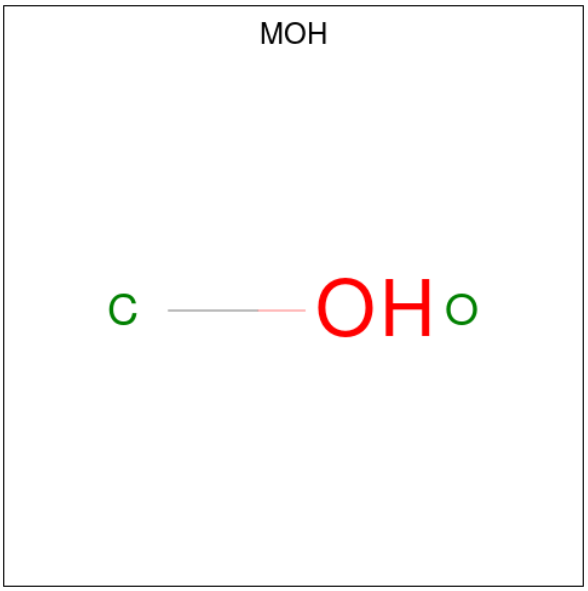
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	21	Total C Mn N O S 58 14 1 17 24 2	0	0
8	B	15	Total C N O S 42 9 12 20 1	0	1
8	C	19	Total C N O S 78 39 5 32 2	0	0
8	D	10	Total C O P 59 29 29 1	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



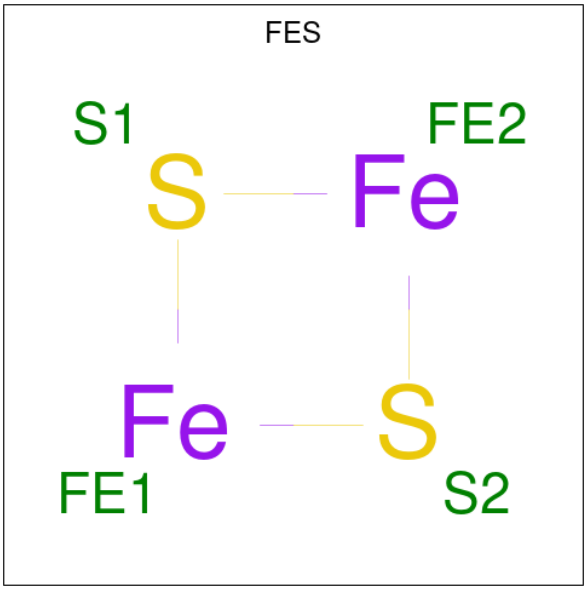
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 5 3 2	0	0

- Molecule 10 is METHANOL (three-letter code: MOH) (formula: CH_4O).



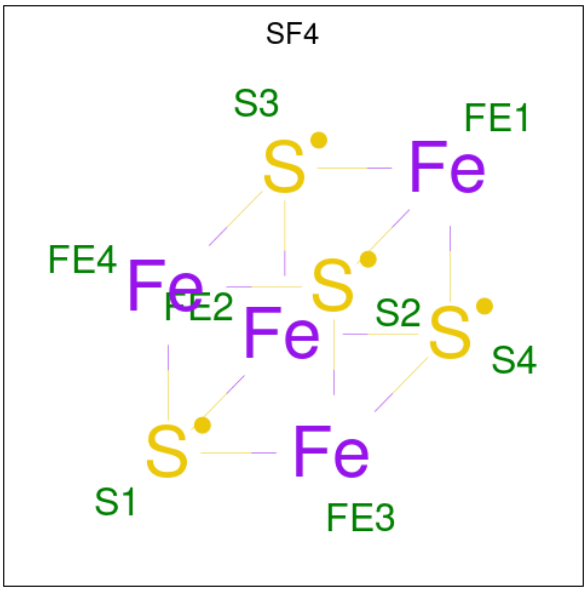
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 2 1 1	0	0

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



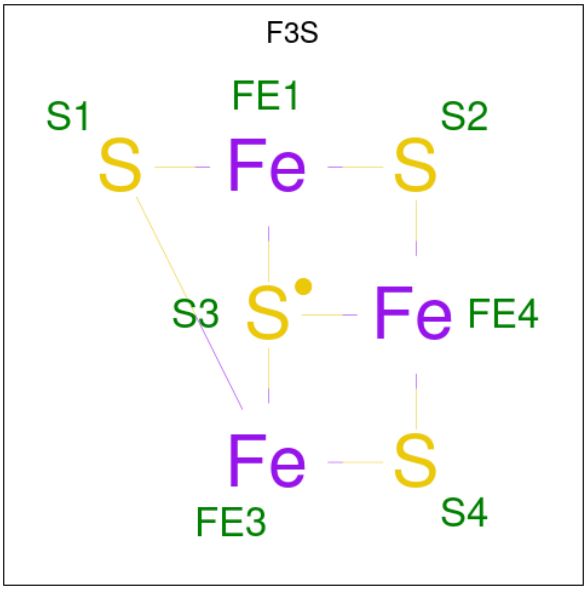
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Fe S 4 2 2	0	0

- Molecule 12 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



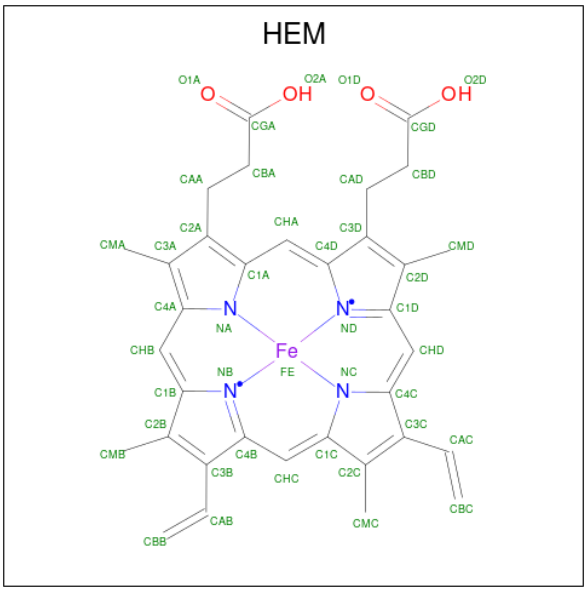
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total Fe S 8 4 4	0	0

- Molecule 13 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



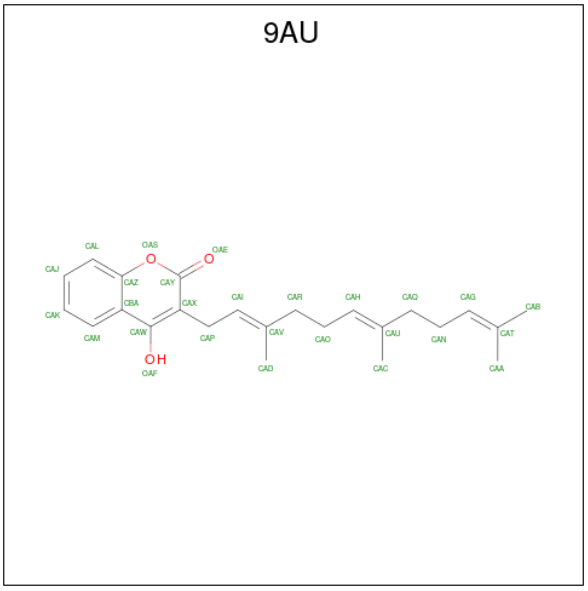
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total Fe S 7 3 4	0	0

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



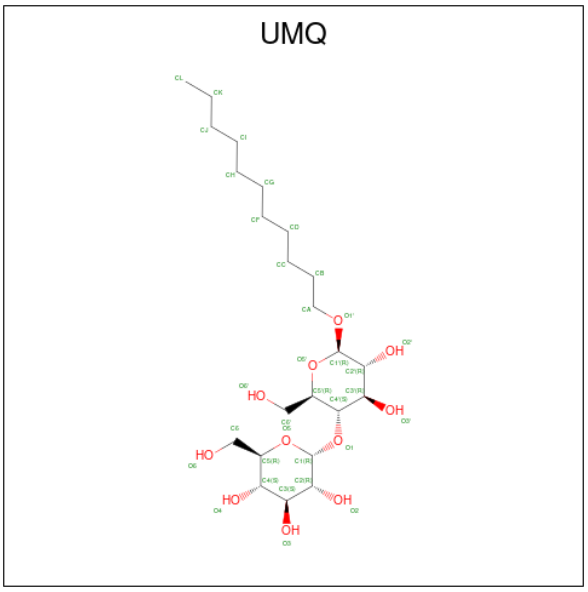
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	0	0
			41	32	1	4	4		

- Molecule 15 is 4-oxidanyl-3-[(2 {E},6 {E})-3,7,11-trimethyldodeca-2,6,10-trienyl]chromen-2-one (three-letter code: 9AU) (formula: $C_{24}H_{30}O_3$) (labeled as "Ligand of Interest" by depositor).



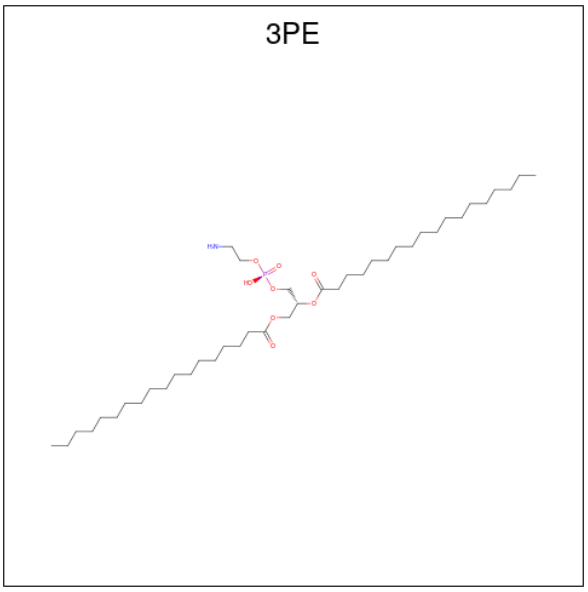
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	O		0	0
			19	16	3			

- Molecule 16 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total C O 34 23 11	0	0

- Molecule 17 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total C N O P 42 32 1 8 1	0	0

- Molecule 18 is water.

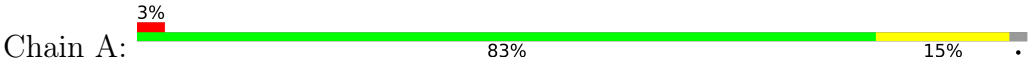
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 2 2	0	1
18	A	234	Total O 237 237	0	3
18	B	145	Total O 146 146	0	1
18	C	1	Total O 2 2	0	1
18	C	1	Total O 1 1	0	0
18	C	51	Total O 51 51	0	0
18	D	31	Total O 31 31	0	0

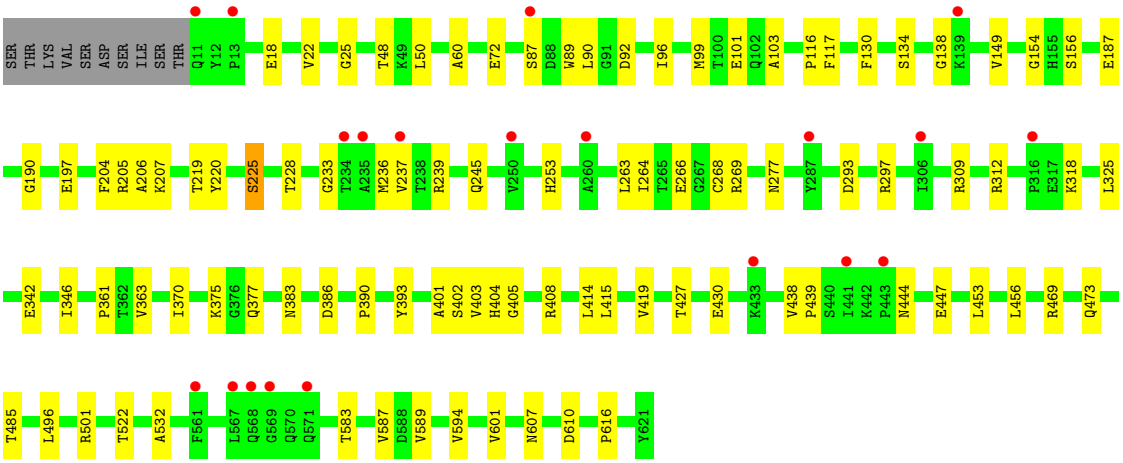
3 Residue-property plots (i)

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

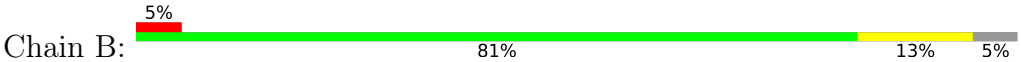
Chain A:

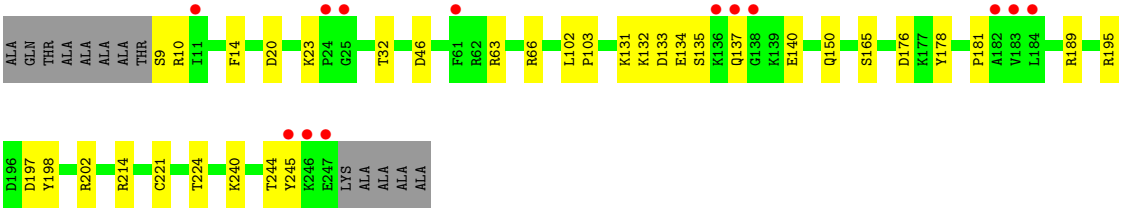




• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

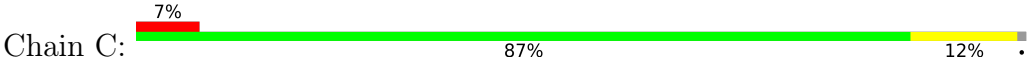
Chain B:

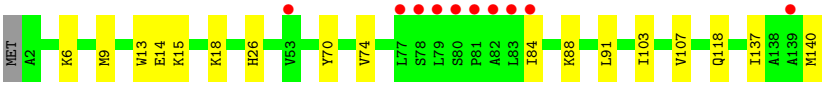




• Molecule 3: Succinate dehydrogenase cytochrome b, large subunit

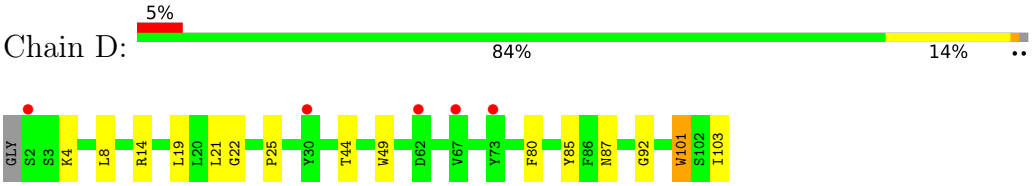
Chain C:





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

Chain D:


5%
84%
14%
GLY
S2
S3
K4
L8
R14
L19
L20
L21
G22
P25
Y30
T44
W49
D62
V67
Y73
F80
Y85
F86
N87
G92
W101
S102
I103

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.91Å 84.55Å 290.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 1.97 29.62 – 1.97	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.62-1.97) 82.9 (29.62-1.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.48 (at 1.96Å)	Xtriage
Refinement program	PHENIX dev_3150	Depositor
R, R_{free}	0.208 , 0.239 0.209 , 0.240	Depositor DCC
R_{free} test set	2334 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9426	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: Y3P, 3PE, SF4, UMQ, F3S, PEG, K, 9AU, MLZ, UNL, FAD, FES, HEM, MOH

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	0.41	0/4824	0.60	0/6531
2	B	0.43	0/1963	0.58	0/2646
3	C	0.38	0/1094	0.54	0/1486
4	D	0.38	0/794	0.50	0/1089
All	All	0.41	0/8675	0.58	0/11752

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	4723	0	4608	67	0
2	B	1921	0	1913	21	0
3	C	1076	0	1116	12	0
4	D	771	0	763	13	0
5	A	53	0	29	5	0
6	A	9	2	0	6	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	58	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	42	0	0	3	0
8	C	78	0	0	1	0
8	D	59	0	0	3	0
9	A	5	0	5	3	0
10	A	2	0	0	1	0
11	B	4	0	0	0	0
12	B	8	0	0	0	0
13	B	7	0	0	0	0
14	C	41	0	24	0	0
15	C	19	0	0	0	0
16	C	34	0	44	0	0
17	D	42	0	61	2	0
18	A	239	0	0	9	0
18	B	146	0	0	3	0
18	C	54	0	0	0	0
18	D	31	0	0	1	0
All	All	9424	2	8563	112	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.

All (112) 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:A:297:ARG:HH22	6:A:1002:Y3P:C3	1.67	1.07
1:A:187:GLU:HG2	1:A:390:PRO:HB2	1.65	0.77
3:C:118:GLN:OE1	8:C:1019:UNL:O	2.11	0.68
4:D:85:TYR:OH	8:D:212:UNL:O	2.12	0.67
1:A:101:GLU:OE2	18:A:1101:HOH:O	2.13	0.67
1:A:297:ARG:HH22	6:A:1002:Y3P:C2	2.10	0.64
1:A:18:GLU:OE2	1:A:205:ARG:NH1	2.31	0.64
1:A:456:LEU:HD13	1:A:522:THR:HG22	1.80	0.62
1:A:50:LEU:HD21	1:A:228:THR:HG21	1.80	0.62
8:D:203:UNL:O5	8:D:203:UNL:O6	2.18	0.61
1:A:25:GLY:HA2	5:A:1001:FAD:H1B	1.83	0.59
2:B:131:LYS:HE3	2:B:195:ARG:O	2.04	0.58
1:A:383:ASN:OD1	8:A:1025:UNL:O	2.21	0.58
18:A:1314:HOH:O	2:B:137:GLN:HG2	2.03	0.58
1:A:239:ARG:HG2	1:A:589:VAL:HG11	1.87	0.57
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.86	0.57
1:A:219:THR:CG2	1:A:532:ALA:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ALA:N	1:A:402:SER:HA	2.19	0.56
1:A:237:VAL:HG21	1:A:370:ILE:HG12	1.86	0.56
1:A:297:ARG:NH2	6:A:1002:Y3P:C3	2.52	0.56
1:A:268:CYS:HB3	1:A:325:LEU:HD21	1.88	0.56
1:A:60:ALA:HA	5:A:1001:FAD:C6	2.35	0.56
3:C:6:LYS:HA	3:C:9:MET:CE	2.36	0.56
1:A:266:GLU:HG3	1:A:269:ARG:NH2	2.22	0.54
1:A:266:GLU:HG3	1:A:269:ARG:CZ	2.38	0.54
9:A:1005:PEG:H41	18:A:1254:HOH:O	2.08	0.54
2:B:198:TYR:O	2:B:202:ARG:HG3	2.07	0.53
1:A:92:ASP:O	1:A:96:ILE:HG13	2.09	0.53
1:A:117:PHE:HA	1:A:149:VAL:HG22	1.91	0.53
3:C:6:LYS:HA	3:C:9:MET:HE2	1.90	0.52
1:A:219:THR:HG21	1:A:532:ALA:HB2	1.90	0.52
1:A:116:PRO:HD2	1:A:156:SER:HB3	1.92	0.52
3:C:74:VAL:HG11	4:D:103:ILE:HD13	1.91	0.52
3:C:84:ILE:HG22	3:C:88:LYS:HE3	1.92	0.51
2:B:140:GLU:HG2	18:B:1165:HOH:O	2.10	0.51
1:A:60:ALA:HA	5:A:1001:FAD:C5X	2.40	0.51
1:A:469:ARG:NE	9:A:1005:PEG:H32	2.25	0.51
1:A:309:ARG:NH1	18:A:1103:HOH:O	2.27	0.50
3:C:137:ILE:HA	3:C:140:MET:HG3	1.92	0.50
1:A:377:GLN:HG2	1:A:393:TYR:CE2	2.46	0.50
9:A:1005:PEG:H31	18:B:1120:HOH:O	2.11	0.50
1:A:22[A]:VAL:HG23	1:A:206:ALA:HB2	1.94	0.49
1:A:99:MET:HA	1:A:419:VAL:HG11	1.95	0.48
1:A:601:VAL:N	8:A:1010:UNL:S2	2.87	0.48
2:B:103:PRO:HB3	3:C:26:HIS:HA	1.96	0.48
1:A:496:LEU:HD12	1:A:496:LEU:HA	1.75	0.47
2:B:9:SER:N	8:B:1014:UNL:O1	2.48	0.47
4:D:44:THR:HG21	4:D:80:PHE:HB2	1.94	0.47
1:A:386:ASP:OD2	18:A:1102:HOH:O	2.20	0.47
4:D:4:LYS:O	4:D:8:LEU:HG	2.13	0.47
4:D:4:LYS:HB3	4:D:4:LYS:HE2	1.73	0.47
1:A:253:HIS:O	1:A:361:PRO:HA	2.15	0.47
1:A:22[A]:VAL:HG23	1:A:206:ALA:CB	2.45	0.47
1:A:269:ARG:HD2	1:A:293:ASP:O	2.15	0.46
4:D:49:TRP:HE1	8:D:203:UNL:C2	2.28	0.46
1:A:233:GLY:HA2	1:A:236:MET:CE	2.45	0.46
4:D:4:LYS:NZ	18:D:304:HOH:O	2.46	0.46
1:A:245:GLN:HA	1:A:583:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLU:O	1:A:346:ILE:HG13	2.16	0.46
2:B:245:TYR:CE1	4:D:4:LYS:HE3	2.51	0.46
2:B:176:ASP:HB3	3:C:13:TRP:CZ2	2.51	0.46
1:A:403:VAL:HG23	1:A:404:HIS:CE1	2.51	0.45
1:A:444:ASN:O	1:A:447:GLU:HB3	2.16	0.45
1:A:225:SER:HB3	18:A:1299:HOH:O	2.16	0.45
2:B:165:SER:HA	2:B:181:PRO:HD2	1.97	0.45
1:A:190:GLY:HA3	1:A:204:PHE:O	2.17	0.45
1:A:501:ARG:HH12	10:A:1011:MOH:C	2.29	0.45
3:C:70:TYR:O	3:C:74:VAL:HG23	2.16	0.45
1:A:220:TYR:CG	1:A:363:VAL:HG21	2.51	0.44
1:A:89:TRP:CE2	1:A:616:PRO:HA	2.53	0.44
1:A:469:ARG:O	1:A:473:GLN:HG3	2.17	0.44
2:B:240:LYS:O	2:B:244:THR:HG23	2.17	0.44
4:D:21:LEU:O	4:D:25:PRO:HD2	2.18	0.44
1:A:438:VAL:HG23	1:A:439:PRO:HD2	2.00	0.44
1:A:297:ARG:HH12	6:A:1002:Y3P:C4	2.31	0.43
1:A:403:VAL:HG22	8:A:1013:UNL:N1	2.32	0.43
2:B:132:LYS:HG2	2:B:197:ASP:HB3	2.00	0.43
1:A:263:LEU:HD22	5:A:1001:FAD:C6	2.49	0.43
2:B:20:ASP:OD2	2:B:23:LYS:NZ	2.31	0.43
3:C:14:GLU:O	3:C:18:LYS:HG2	2.18	0.43
4:D:22:GLY:O	4:D:25:PRO:HG2	2.19	0.43
2:B:14:PHE:O	2:B:32:THR:HA	2.18	0.43
1:A:375:LYS:HA	18:A:1141:HOH:O	2.16	0.43
1:A:277:ASN:ND2	1:A:312:ARG:HD2	2.34	0.43
2:B:133:ASP:OD1	2:B:135:SER:OG	2.37	0.43
2:B:178:TYR:CD1	2:B:214:ARG:HB2	2.53	0.43
1:A:87:SER:HB2	1:A:405:GLY:HA3	1.99	0.43
1:A:103:ALA:HB2	1:A:415:LEU:HD21	2.00	0.43
3:C:103:ILE:O	3:C:107:VAL:HG23	2.18	0.43
2:B:10:ARG:NH2	18:B:1112:HOH:O	2.38	0.43
1:A:297:ARG:HH22	6:A:1002:Y3P:C4	2.27	0.42
1:A:427:THR:HA	1:A:430:GLU:HG2	2.01	0.42
2:B:102:LEU:HA	2:B:103:PRO:HD3	1.88	0.42
4:D:101:TRP:CE2	17:D:201:3PE:H322	2.55	0.42
1:A:414:LEU:HG	5:A:1001:FAD:C2	2.50	0.42
3:C:91:LEU:HD23	3:C:91:LEU:HA	1.94	0.42
2:B:137:GLN:HG3	8:B:1019:UNL:O	2.20	0.42
1:A:263:LEU:HG	1:A:264:ILE:N	2.34	0.41
1:A:587:VAL:HG22	1:A:594:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:87:ASN:HA	4:D:92:GLY:HA2	2.02	0.41
1:A:607:ASN:ND2	1:A:610:ASP:HB2	2.35	0.41
1:A:90:LEU:HD12	1:A:601:VAL:CG2	2.51	0.41
2:B:221:CYS:O	2:B:224:THR:HG22	2.20	0.41
1:A:318:LYS:HE3	1:A:318:LYS:HB3	1.81	0.41
1:A:134:SER:OG	1:A:138:GLY:HA2	2.21	0.41
4:D:101:TRP:CD2	17:D:201:3PE:H322	2.56	0.41
2:B:46:ASP:HB3	8:B:1013:UNL:C1	2.51	0.40
1:A:90:LEU:HD12	1:A:601:VAL:HG21	2.02	0.40
2:B:131:LYS:O	2:B:134:GLU:HG3	2.21	0.40
1:A:197:GLU:HB2	18:A:1106:HOH:O	2.22	0.40
1:A:197:GLU:HB3	18:A:1193[A]:HOH:O	2.21	0.40
1:A:408:ARG:NH1	6:A:1002:Y3P:O5	2.39	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	610/621 (98%)	590 (97%)	20 (3%)	0	100	100
2	B	237/252 (94%)	232 (98%)	5 (2%)	0	100	100
3	C	136/140 (97%)	135 (99%)	1 (1%)	0	100	100
4	D	100/103 (97%)	98 (98%)	2 (2%)	0	100	100
All	All	1083/1116 (97%)	1055 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	489 (99%)	7 (1%)	67 62
2	B	215/219 (98%)	211 (98%)	4 (2%)	57 50
3	C	116/117 (99%)	116 (100%)	0	100 100
4	D	78/79 (99%)	75 (96%)	3 (4%)	33 21
All	All	905/921 (98%)	891 (98%)	14 (2%)	65 59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	THR
1	A	72	GLU
1	A	130	PHE
1	A	207	LYS
1	A	225	SER
1	A	453	LEU
1	A	485	THR
2	B	63	ARG
2	B	66	ARG
2	B	150	GLN
2	B	189	ARG
4	D	14	ARG
4	D	19	LEU
4	D	101	TRP

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

Mol	Chain	Res	Type
2	B	150	GLN
3	C	118	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
3	MLZ	C	15	3	8,9,10	0.61	0	4,9,11	1.74	1 (25%)

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
3	MLZ	C	15	3	-	2/7/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	15	MLZ	CM-NZ-CE	3.29	121.45	111.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	15	MLZ	CG-CD-CE-NZ
3	C	15	MLZ	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 79 ligands modelled in this entry, 2 are monoatomic and 66 are unknown - leaving 11 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	$\#\|Z\| > 2$
14	HEM	C	201	4,3	40,48,50	1.44	6 (15%)	46,80,82	1.73	10 (21%)
17	3PE	D	201	-	41,41,50	1.09	2 (4%)	44,46,55	1.09	4 (9%)
6	Y3P	A	1002	-	8,8,8	2.65	4 (50%)	9,10,10	2.46	4 (44%)
9	PEG	A	1005	-	4,4,6	0.59	0	3,3,5	0.12	0
10	MOH	A	1011	-	1,1,1	0.07	0	-		
11	FES	B	1001	2	0,4,4	-	-	-		
16	UMQ	C	1002	-	35,35,35	0.55	0	46,46,46	0.91	2 (4%)
13	F3S	B	1003	2	0,9,9	-	-	-		
12	SF4	B	1002	2	0,12,12	-	-	-		
5	FAD	A	1001	1	53,58,58	0.80	1 (1%)	68,89,89	1.33	7 (10%)
15	9AU	C	202	-	20,20,28	2.95	8 (40%)	24,27,37	2.08	10 (41%)

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
14	HEM	C	201	4,3	-	3/10/50/54	-
17	3PE	D	201	-	-	16/45/45/54	-
6	Y3P	A	1002	-	-	4/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PEG	A	1005	-	-	0/2/2/4	-
11	FES	B	1001	2	-	-	0/1/1/1
16	UMQ	C	1002	-	-	8/20/60/60	0/2/2/2
13	F3S	B	1003	2	-	-	0/3/3/3
12	SF4	B	1002	2	-	-	0/6/5/5
5	FAD	A	1001	1	-	5/30/50/50	0/6/6/6
15	9AU	C	202	-	-	3/8/8/17	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	202	9AU	OAS-CAZ	7.69	1.50	1.38
6	A	1002	Y3P	C2-C1	5.59	1.55	1.48
15	C	202	9AU	CAW-CAX	5.55	1.48	1.36
15	C	202	9AU	OAS-CAY	5.13	1.45	1.38
17	D	201	3PE	O21-C21	4.59	1.47	1.34
17	D	201	3PE	O31-C31	4.37	1.46	1.33
15	C	202	9AU	CAP-CAI	3.73	1.56	1.50
14	C	201	HEM	FE-ND	3.23	2.12	1.96
15	C	202	9AU	CBA-CAW	3.18	1.50	1.45
15	C	202	9AU	OAF-CAW	3.08	1.41	1.33
15	C	202	9AU	CAP-CAX	2.93	1.56	1.51
6	A	1002	Y3P	O4-C4	2.64	1.29	1.23
14	C	201	HEM	C2C-C3C	-2.43	1.33	1.41
15	C	202	9AU	CAR-CAV	2.33	1.56	1.51
6	A	1002	Y3P	O3-C2	2.29	1.39	1.34
5	A	1001	FAD	C4-N3	-2.24	1.34	1.38
14	C	201	HEM	CMC-C2C	2.21	1.56	1.51
14	C	201	HEM	CMB-C2B	2.14	1.55	1.50
14	C	201	HEM	C1A-NA	2.07	1.40	1.36
6	A	1002	Y3P	O1-C1	-2.04	1.24	1.30
14	C	201	HEM	FE-NB	2.02	2.06	1.96

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	202	9AU	CAZ-OAS-CAY	-4.73	117.62	122.23
14	C	201	HEM	C4B-CHC-C1C	4.33	128.28	122.56
6	A	1002	Y3P	O2-C1-C2	-4.31	115.11	120.08
6	A	1002	Y3P	O1-C1-C2	4.09	119.85	115.91
5	A	1001	FAD	C4-N3-C2	-3.78	118.66	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	D	201	3PE	O21-C21-C22	3.74	119.56	111.50
14	C	201	HEM	C1B-NB-C4B	3.65	108.84	105.07
17	D	201	3PE	O31-C31-C32	3.35	122.43	111.91
6	A	1002	Y3P	O3-C2-C1	3.27	115.99	114.01
5	A	1001	FAD	C4X-C4-N3	3.27	121.48	113.19
14	C	201	HEM	CBA-CAA-C2A	-3.11	107.32	112.62
15	C	202	9AU	CAD-CAV-CAR	3.09	120.47	115.27
15	C	202	9AU	CAZ-CBA-CAW	3.05	120.60	117.79
15	C	202	9AU	OAS-CAZ-CAL	3.01	120.24	116.26
15	C	202	9AU	CAO-CAR-CAV	-3.00	109.72	114.62
15	C	202	9AU	OAS-CAY-OAE	2.99	120.17	116.22
14	C	201	HEM	C3B-C4B-NB	-2.97	106.33	109.88
14	C	201	HEM	C4D-ND-C1D	2.93	108.10	105.07
15	C	202	9AU	CAP-CAI-CAV	-2.84	122.06	126.79
5	A	1001	FAD	O4-C4-C4X	-2.76	119.28	126.60
17	D	201	3PE	O31-C31-O32	-2.66	116.89	123.59
15	C	202	9AU	CAM-CBA-CAW	-2.60	118.02	122.50
14	C	201	HEM	CAD-CBD-CGD	-2.59	108.02	113.60
14	C	201	HEM	C4B-C3B-C2B	2.58	109.44	107.07
14	C	201	HEM	C4C-CHD-C1D	2.48	125.83	122.56
5	A	1001	FAD	C4-C4X-N5	2.48	121.76	118.23
15	C	202	9AU	CAM-CBA-CAZ	2.42	121.38	118.21
16	C	1002	UMQ	O5-C5-C6	2.40	112.40	106.44
5	A	1001	FAD	O2-C2-N1	-2.33	117.97	121.83
14	C	201	HEM	CMA-C3A-C4A	-2.31	124.92	128.46
16	C	1002	UMQ	O5'-C5'-C6'	2.20	111.90	106.44
5	A	1001	FAD	O5'-C5'-C4'	-2.20	103.50	109.36
15	C	202	9AU	OAE-CAY-CAX	-2.14	120.59	125.30
14	C	201	HEM	CHD-C1D-ND	2.13	126.75	124.43
17	D	201	3PE	C3-C2-C1	-2.12	106.77	111.79
5	A	1001	FAD	O5B-C5B-C4B	-2.06	101.91	108.99
6	A	1002	Y3P	O4-C4-C3	-2.00	117.52	123.89

There are no chirality outliers.

All (39) 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'
6	A	1002	Y3P	O1-C1-C2-O3
6	A	1002	Y3P	O2-C1-C2-O3
17	D	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
17	D	201	3PE	C22-C21-O21-C2
17	D	201	3PE	O22-C21-O21-C2
16	C	1002	UMQ	C2-C1-O1-C4'
16	C	1002	UMQ	O1'-CA-CB-CC
17	D	201	3PE	C32-C33-C34-C35
16	C	1002	UMQ	O5-C1-O1-C4'
15	C	202	9AU	CAH-CAO-CAR-CAV
16	C	1002	UMQ	CF-CG-CH-CI
17	D	201	3PE	C21-C22-C23-C24
16	C	1002	UMQ	CG-CH-CI-CJ
16	C	1002	UMQ	CC-CD-CF-CG
5	A	1001	FAD	PA-O3P-P-O5'
17	D	201	3PE	C2B-C2C-C2D-C2E
15	C	202	9AU	CAO-CAR-CAV-CAD
15	C	202	9AU	CAO-CAR-CAV-CAI
17	D	201	3PE	C36-C37-C38-C39
17	D	201	3PE	C2F-C2G-C2H-C2I
6	A	1002	Y3P	O1-C1-C2-C3
6	A	1002	Y3P	O2-C1-C2-C3
14	C	201	HEM	C2A-CAA-CBA-CGA
16	C	1002	UMQ	CD-CF-CG-CH
17	D	201	3PE	C34-C35-C36-C37
17	D	201	3PE	C1-O11-P-O13
17	D	201	3PE	C32-C31-O31-C3
14	C	201	HEM	CAA-CBA-CGA-O2A
17	D	201	3PE	C2E-C2F-C2G-C2H
16	C	1002	UMQ	CA-CB-CC-CD
14	C	201	HEM	CAA-CBA-CGA-O1A
17	D	201	3PE	O32-C31-O31-C3
5	A	1001	FAD	O4B-C4B-C5B-O5B
5	A	1001	FAD	P-O3P-PA-O2A
17	D	201	3PE	C2D-C2E-C2F-C2G
17	D	201	3PE	O31-C31-C32-C33
17	D	201	3PE	C2-C1-O11-P

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	201	3PE	2	0
6	A	1002	Y3P	6	0
9	A	1005	PEG	3	0

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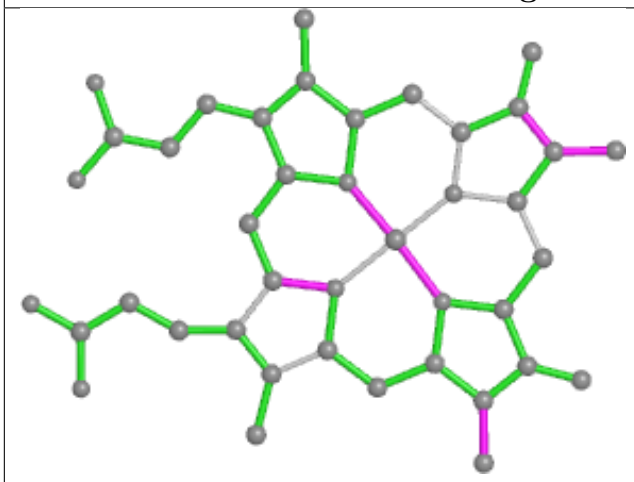
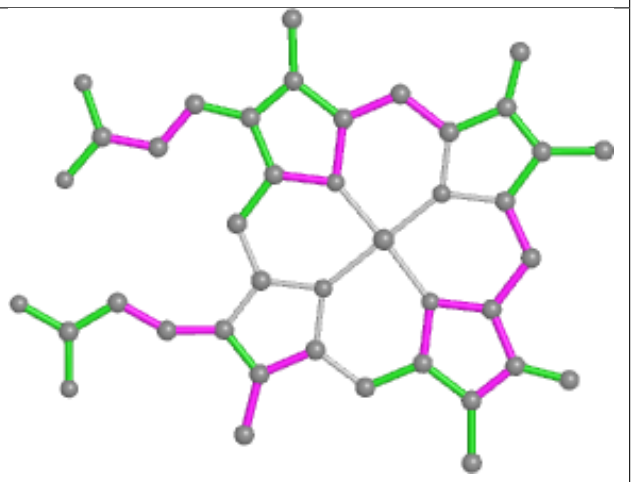
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1011	MOH	1	0
5	A	1001	FAD	5	0

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

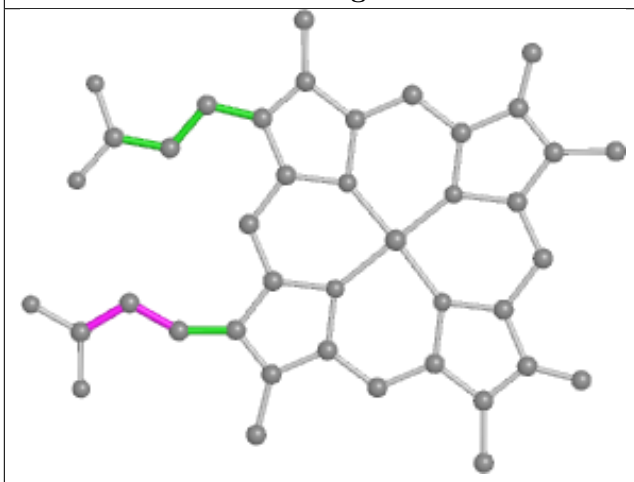
Ligand HEM C 201



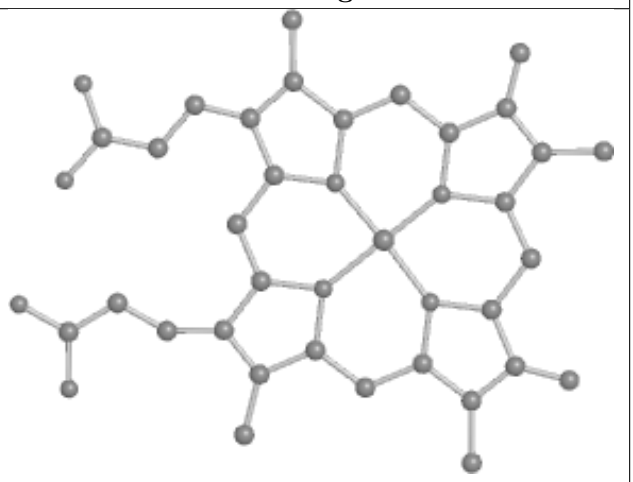
Bond lengths



Bond angles

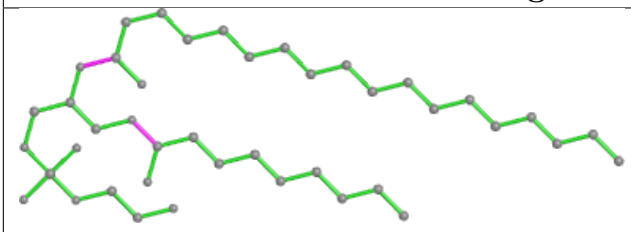


Torsions

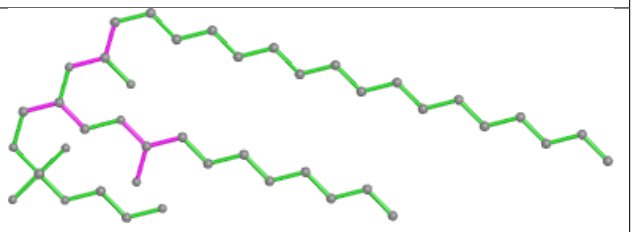


Rings

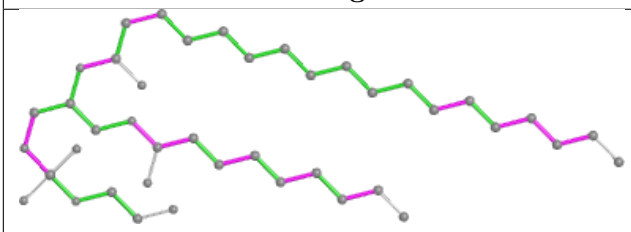
Ligand 3PE D 201



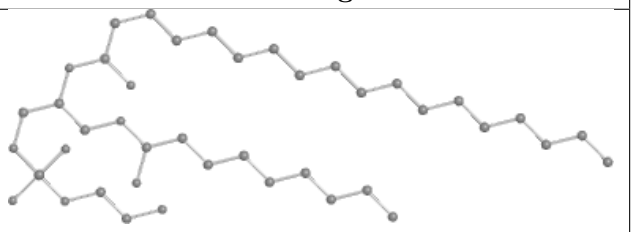
Bond lengths



Bond angles

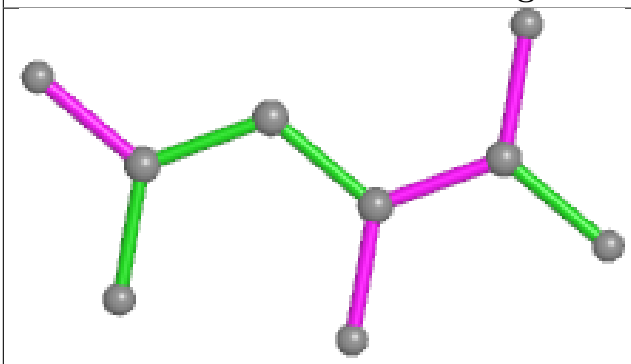


Torsions

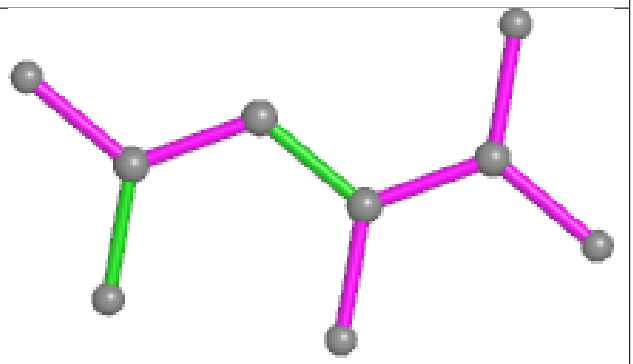


Rings

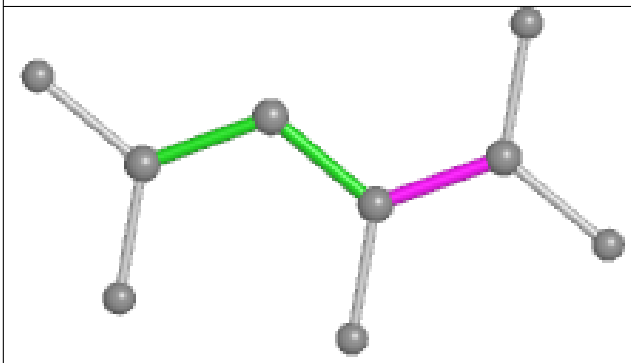
Ligand Y3P A 1002



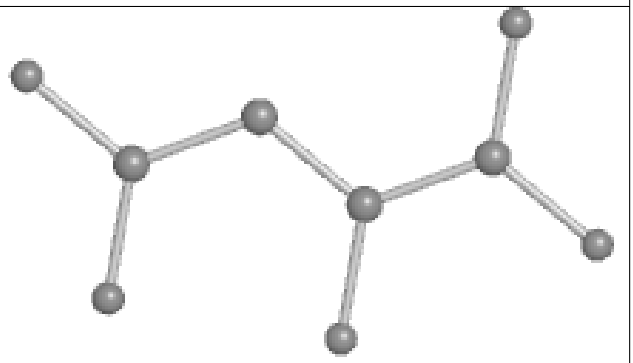
Bond lengths



Bond angles

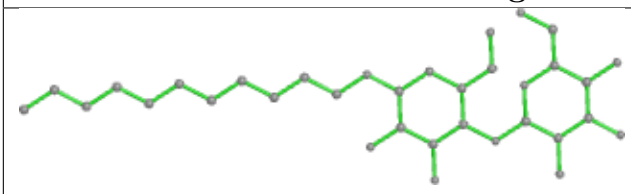


Torsions

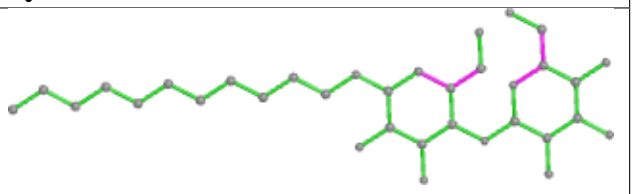


Rings

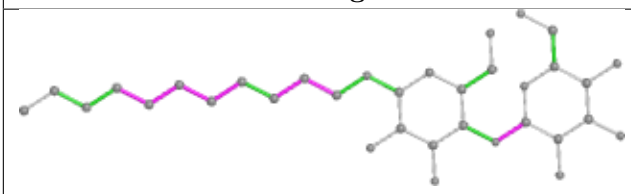
Ligand UMQ C 1002



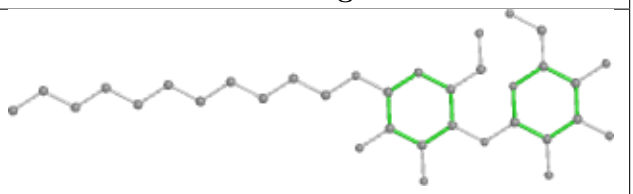
Bond lengths



Bond angles

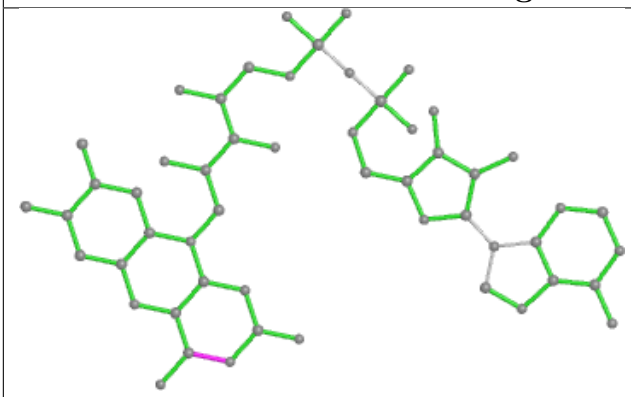


Torsions

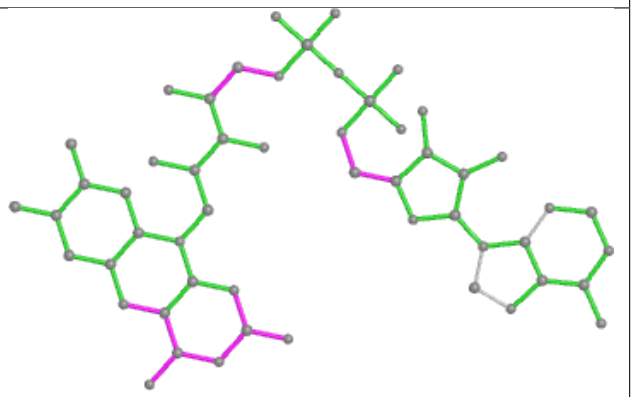


Rings

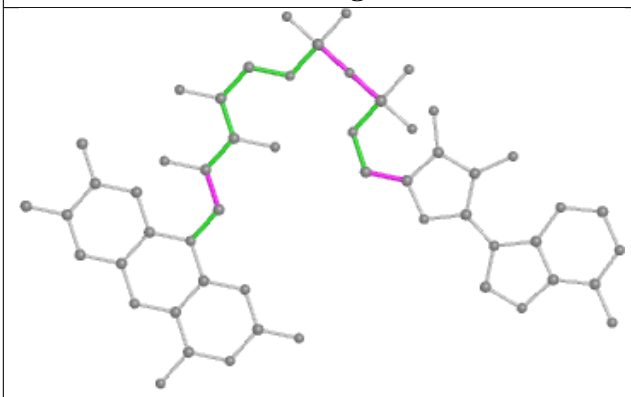
Ligand FAD A 1001



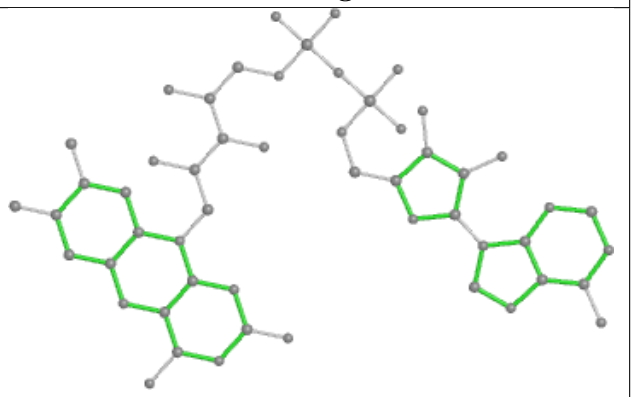
Bond lengths



Bond angles

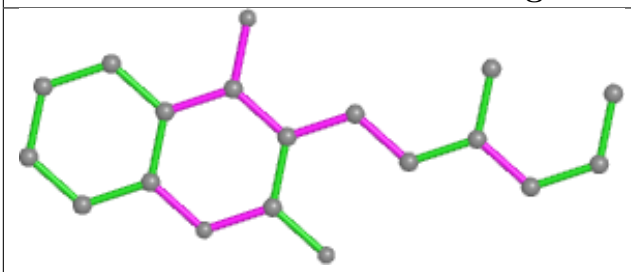


Torsions

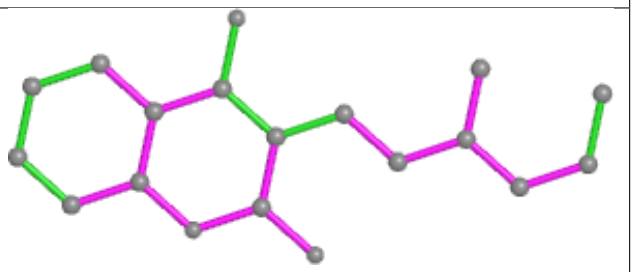


Rings

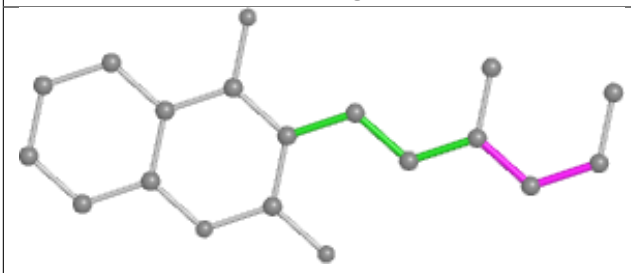
Ligand 9AU C 202



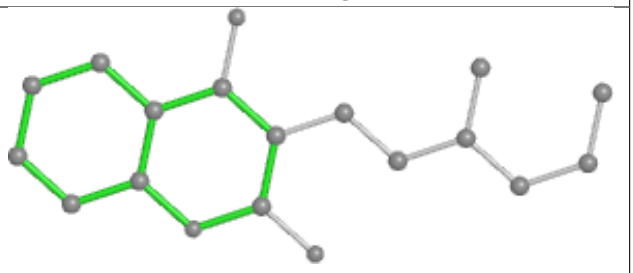
Bond lengths



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	611/621 (98%)	0.31	20 (3%) 46 49	32, 51, 75, 101	0
2	B	239/252 (94%)	0.34	13 (5%) 25 28	31, 42, 71, 89	0
3	C	138/140 (98%)	0.52	10 (7%) 15 17	35, 48, 74, 81	0
4	D	102/103 (99%)	0.44	5 (4%) 29 32	36, 48, 66, 86	0
All	All	1090/1116 (97%)	0.36	48 (4%) 34 36	31, 49, 73, 101	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	79	LEU	7.6
3	C	81	PRO	4.5
4	D	30	TYR	4.2
1	A	567	LEU	4.2
2	B	25	GLY	4.1
3	C	84	ILE	4.0
3	C	83	LEU	3.9
2	B	245	TYR	3.9
3	C	82	ALA	3.8
3	C	139	ALA	3.8
2	B	24	PRO	3.7
2	B	246	LYS	3.3
1	A	433	LYS	3.1
3	C	53	VAL	3.1
1	A	250	VAL	3.0
2	B	136	LYS	2.9
1	A	443	PRO	2.9
1	A	306	ILE	2.9
3	C	77	LEU	2.9
4	D	2	SER	2.9
2	B	11	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	78	SER	2.8
1	A	568	GLN	2.8
1	A	561	PHE	2.7
1	A	11	GLN	2.7
2	B	182	ALA	2.6
1	A	237	VAL	2.6
2	B	183	VAL	2.6
1	A	13	PRO	2.5
2	B	61	PHE	2.5
1	A	569	GLY	2.5
2	B	138	GLY	2.5
2	B	184	LEU	2.5
1	A	316	PRO	2.4
2	B	247	GLU	2.4
1	A	287	TYR	2.3
1	A	139	LYS	2.3
1	A	234	THR	2.2
3	C	80	SER	2.2
1	A	441	ILE	2.1
1	A	235	ALA	2.1
1	A	571	GLN	2.1
4	D	73	TYR	2.1
4	D	67	VAL	2.1
4	D	62	ASP	2.1
2	B	137	GLN	2.1
1	A	260	ALA	2.0
1	A	87	SER	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, 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
3	MLZ	C	15	10/11	0.94	0.12	50,59,65,65	0

6.3 Carbohydrates (i)

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
8	UNL	D	207	12/-	0.58	0.43	75,81,89,90	0
8	UNL	D	211	1/-	0.61	0.18	61,61,61,61	0
8	UNL	C	1021	1/-	0.64	0.47	60,60,60,60	0
8	UNL	C	1022	1/-	0.65	0.18	66,66,66,66	0
8	UNL	A	1023	1/-	0.70	0.20	72,72,72,72	0
8	UNL	B	1016	1/-	0.70	0.18	59,59,59,59	0
17	3PE	D	201	42/51	0.70	0.28	66,82,115,119	0
8	UNL	A	1012	2/-	0.72	0.23	70,70,70,71	0
8	UNL	C	1005	15/-	0.73	0.39	52,72,78,78	15
8	UNL	C	1018	1/-	0.74	0.17	57,57,57,57	0
8	UNL	A	1027	1/-	0.75	0.48	49,49,49,49	1
8	UNL	A	1025	1/-	0.76	0.20	73,73,73,73	0
8	UNL	B	1009	3/-	0.76	0.40	42,42,43,46	3
8	UNL	D	212	1/-	0.77	0.68	63,63,63,63	0
8	UNL	D	206	5/-	0.78	0.37	74,74,79,79	0
8	UNL	B	1017	1/-	0.79	0.18	47,47,47,47	0
8	UNL	C	1007	5/-	0.79	0.19	54,55,60,62	0
10	MOH	A	1011	2/2	0.80	0.41	79,79,79,81	0
8	UNL	B	1012	2/-	0.80	0.38	85,85,85,86	0
8	UNL	C	1006	12/-	0.81	0.16	63,73,75,75	0
8	UNL	A	1020	3/-	0.81	0.26	39,39,46,53	0
8	UNL	C	1010	15/-	0.81	0.41	74,76,93,94	15
8	UNL	B	1014	4/-	0.82	0.23	89,91,91,92	0
8	UNL	C	1009	4/-	0.82	0.24	75,75,76,76	0
9	PEG	A	1005	5/7	0.83	0.40	67,67,72,74	0
8	UNL	A	1021	3/-	0.83	0.21	44,44,60,64	0
8	UNL	A	1022	1/-	0.83	0.18	76,76,76,76	0
8	UNL	A	1017	2/-	0.84	0.57	80,80,80,82	0
8	UNL	B	1006	3/-	0.84	0.20	64,64,66,67	0
8	UNL	B	1007	3/-	0.84	0.13	58,58,65,65	0
8	UNL	A	1010	4/-	0.84	0.15	68,68,72,80	0
8	UNL	B	1011	4/-	0.84	0.16	69,73,74,78	0
15	9AU	C	202	19/27	0.84	0.26	38,57,67,69	0
8	UNL	A	1016	2/-	0.84	0.13	64,64,64,64	0
8	UNL	B	1013	4/-	0.85	0.21	45,46,47,50	4
8	UNL	C	1003	3/-	0.85	0.19	47,47,52,56	0
8	UNL	D	205	1/-	0.85	0.20	65,65,65,65	0

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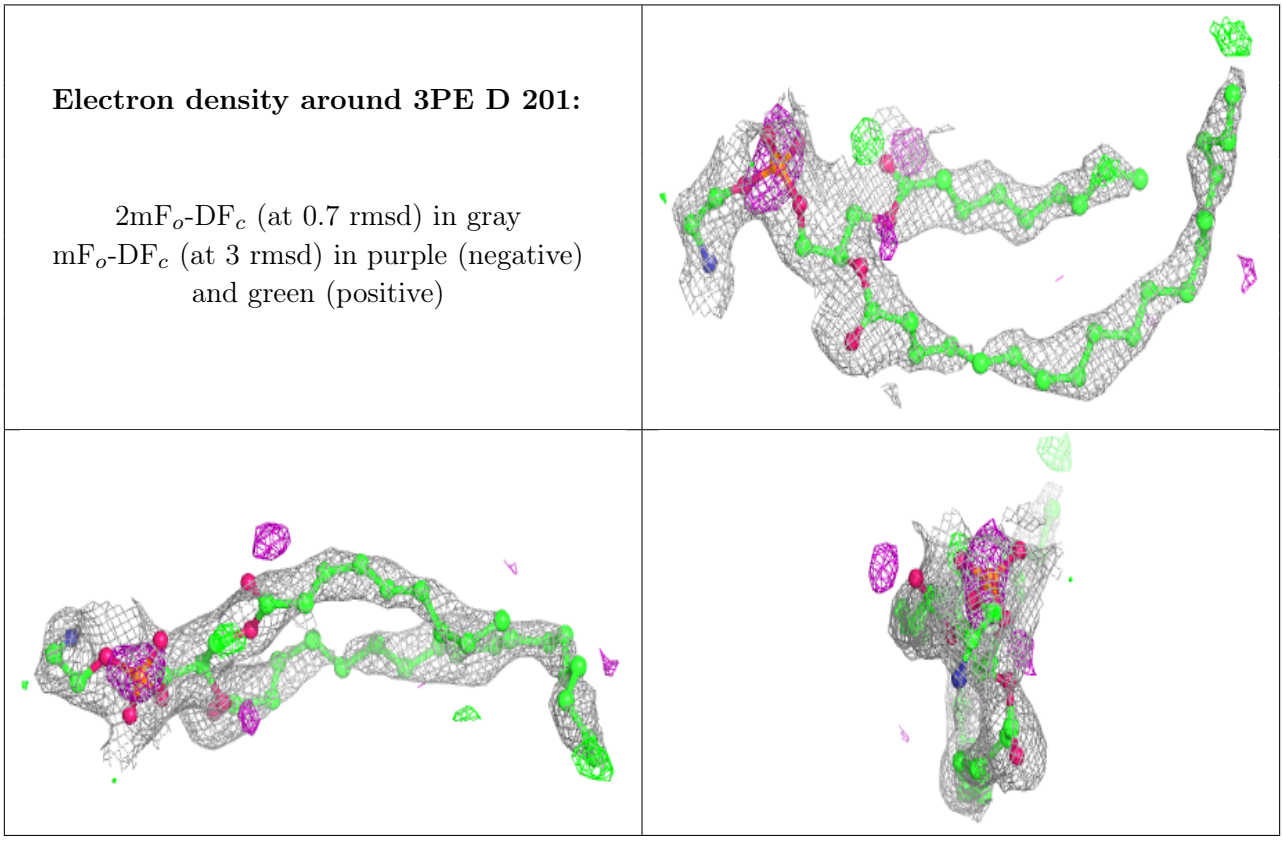
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	UNL	A	1018	2/-	0.85	0.33	53,53,53,60	0
8	UNL	A	1013	3/-	0.85	0.26	37,37,37,49	3
8	UNL	D	208	12/-	0.85	0.23	72,76,79,80	0
8	UNL	C	1016	1/-	0.86	0.21	55,55,55,55	0
8	UNL	D	203	11/-	0.86	0.17	56,74,78,79	0
8	UNL	C	1017	1/-	0.86	0.15	54,54,54,54	0
8	UNL	D	210	1/-	0.87	0.10	45,45,45,45	0
8	UNL	C	1015	1/-	0.88	0.13	44,44,44,44	0
8	UNL	C	1019	1/-	0.88	0.19	53,53,53,53	0
8	UNL	C	1008	3/-	0.88	0.28	51,51,59,60	0
8	UNL	C	1011	4/-	0.88	0.28	67,67,71,80	0
8	UNL	B	1010	6/-	0.89	0.30	61,64,65,67	6
8	UNL	B	1018[A]	1/-	0.89	0.27	29,29,29,29	1
8	UNL	B	1018[B]	1/-	0.89	0.27	28,28,28,28	1
8	UNL	B	1019	1/-	0.90	0.37	56,56,56,56	0
8	UNL	B	1015	1/-	0.90	0.35	64,64,64,64	0
8	UNL	D	209	10/-	0.91	0.16	60,70,71,73	0
16	UMQ	C	1002	34/34	0.91	0.23	40,61,78,83	0
8	UNL	A	1024	1/-	0.91	0.19	48,48,48,48	0
8	UNL	B	1005	4/-	0.92	0.12	51,54,57,63	0
8	UNL	C	1012	3/-	0.92	0.30	73,73,74,76	0
8	UNL	C	1013	3/-	0.92	0.10	68,68,68,68	0
8	UNL	A	1007	4/-	0.92	0.13	69,71,73,76	0
8	UNL	D	204	5/-	0.93	0.29	45,48,49,51	5
8	UNL	A	1019	3/-	0.93	0.15	64,64,66,66	0
8	UNL	A	1026	1/-	0.93	0.25	56,56,56,56	0
8	UNL	A	1015	3/-	0.93	0.14	65,65,68,69	0
8	UNL	C	1014	1/-	0.93	0.13	49,49,49,49	0
8	UNL	C	1004	3/-	0.93	0.13	50,50,52,54	0
8	UNL	A	1006	7/-	0.93	0.16	68,70,71,72	0
8	UNL	A	1008	4/-	0.94	0.10	63,66,67,69	0
8	UNL	B	1008	3/-	0.94	0.12	40,40,50,53	0
8	UNL	A	1004	6/-	0.95	0.15	66,67,69,77	4
6	Y3P	A	1002	9/9	0.95	0.13	41,53,64,66	0
8	UNL	A	1009	4/-	0.95	0.09	65,65,66,73	0
7	K	B	1004	1/1	0.97	0.17	84,84,84,84	0
12	SF4	B	1002	8/8	0.97	0.11	30,36,41,41	0
14	HEM	C	201	41/43	0.97	0.18	34,42,51,53	0
5	FAD	A	1001	53/53	0.98	0.13	32,39,46,49	0
7	K	A	1003	1/1	0.99	0.09	53,53,53,53	0
13	F3S	B	1003	7/7	0.99	0.15	31,35,36,36	0
11	FES	B	1001	4/4	0.99	0.10	36,38,38,39	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.

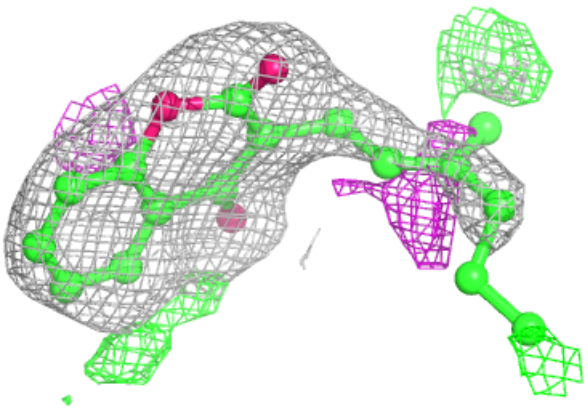
Electron density around 3PE D 201:

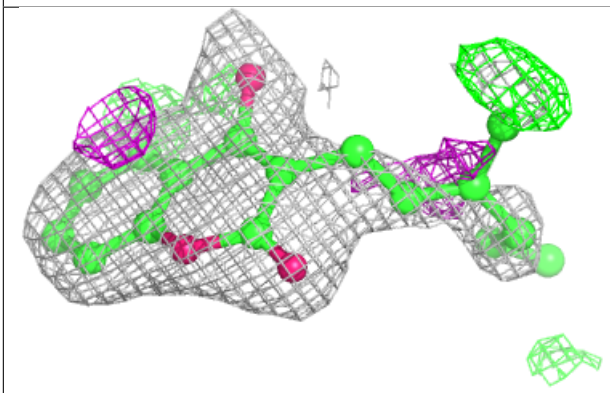
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

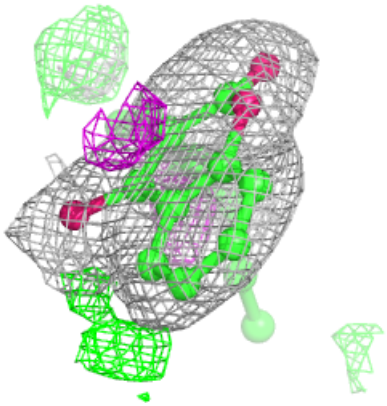


Electron density around 9AU C 202:

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

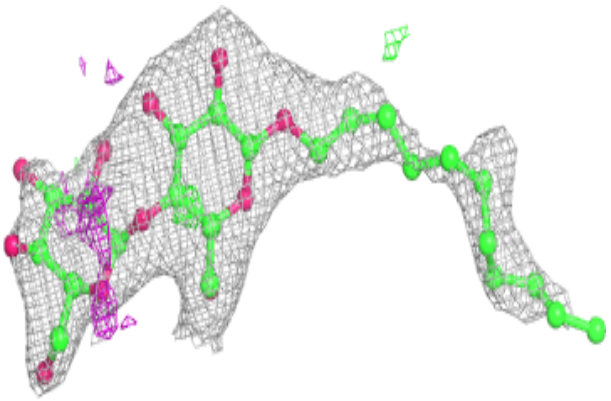


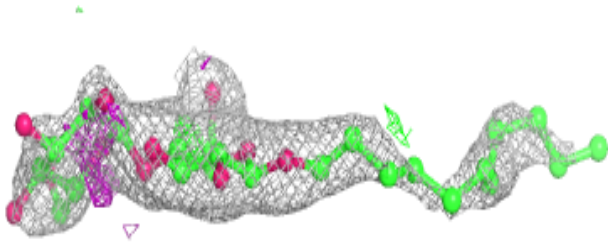


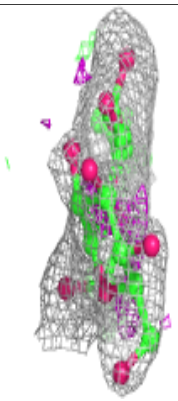


Electron density around UMQ C 1002:

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

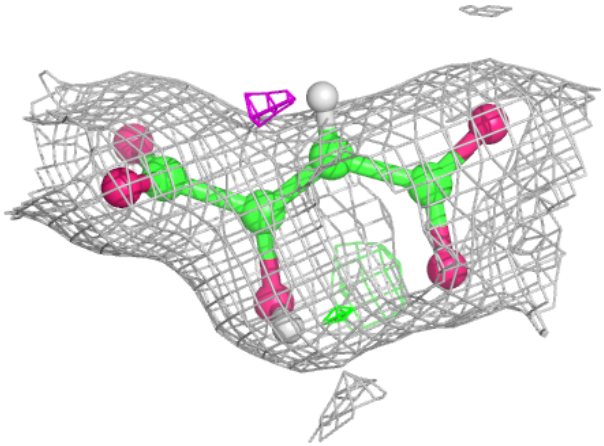


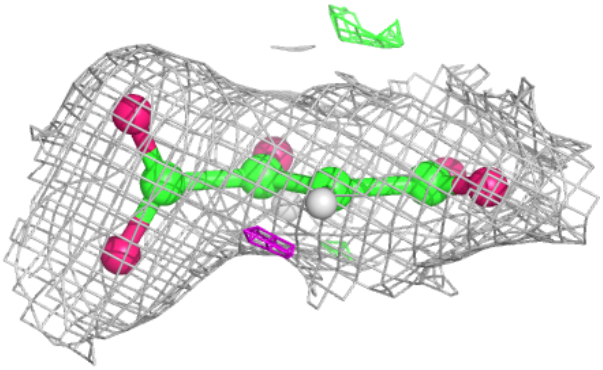


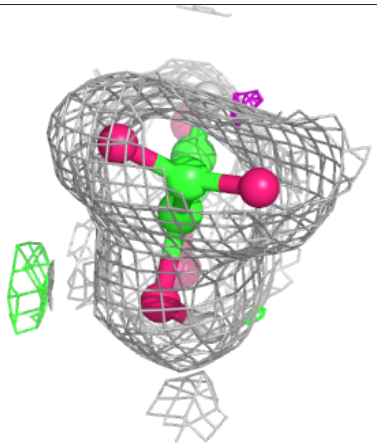


Electron density around Y3P A 1002:

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

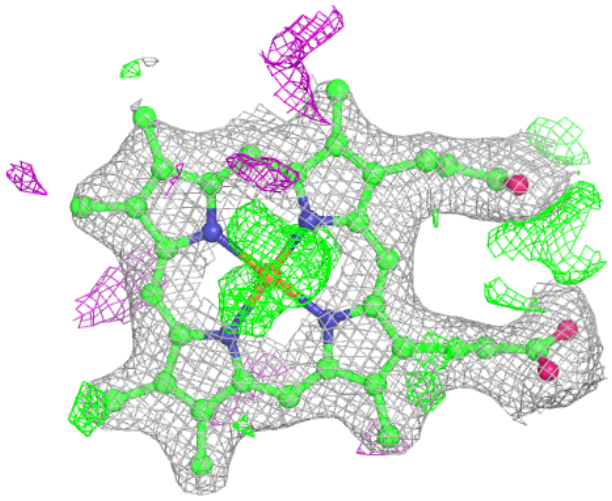


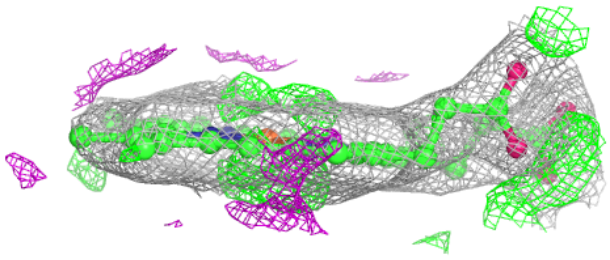


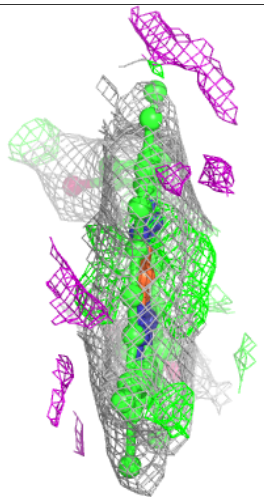


Electron density around HEM C 201:

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

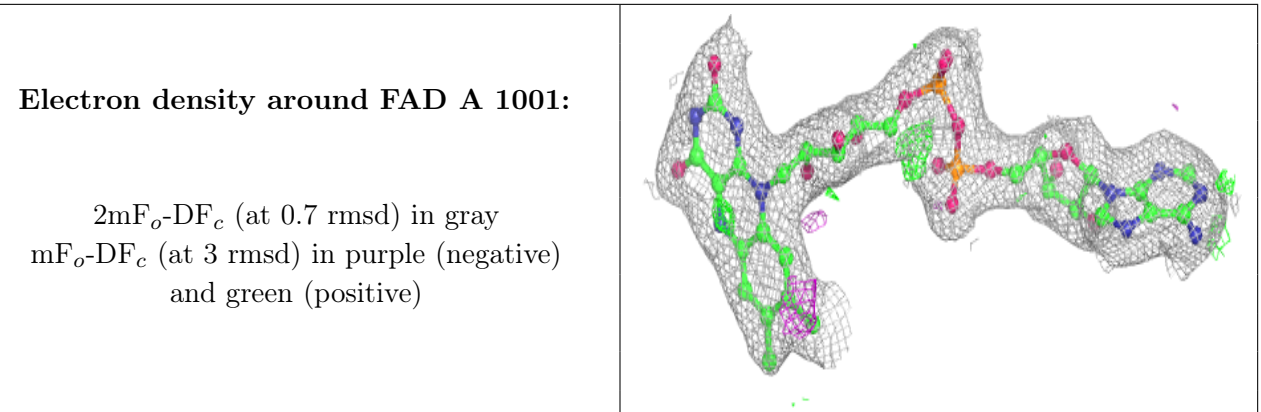


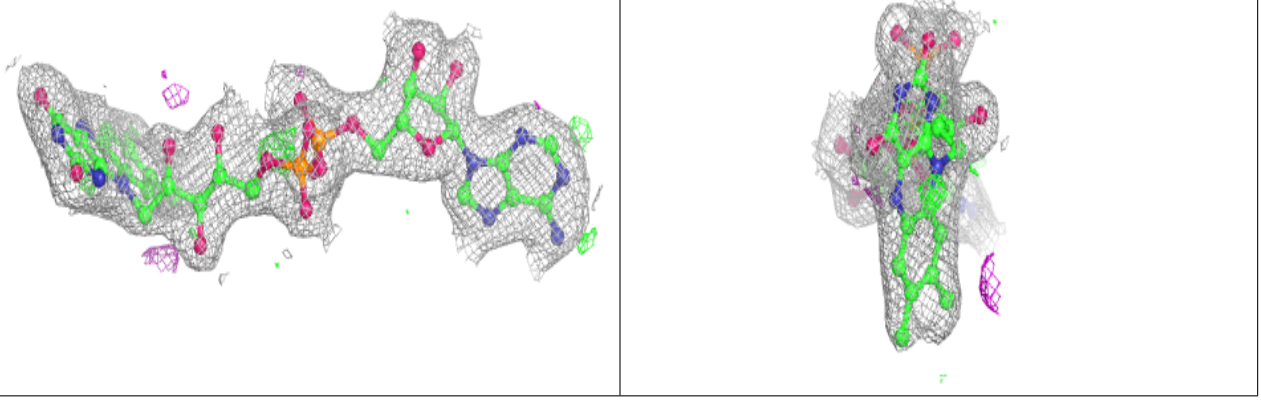




Electron density around FAD A 1001:

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





6.5 Other polymers (i)

There are no such residues in this entry.