wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 02:39 AM EDT

PDB ID	:	1L0V
Title	:	Quinol-Fumarate Reductase with Menaquinol Molecules
Authors	:	Iverson, T.M.; Luna-Chavez, C.; Croal, L.R.; Cecchini, G.; Rees, D.C.
Deposited on	:	2002-02-13
Resolution	:	3.30 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 (1)) were used in the production of this report:

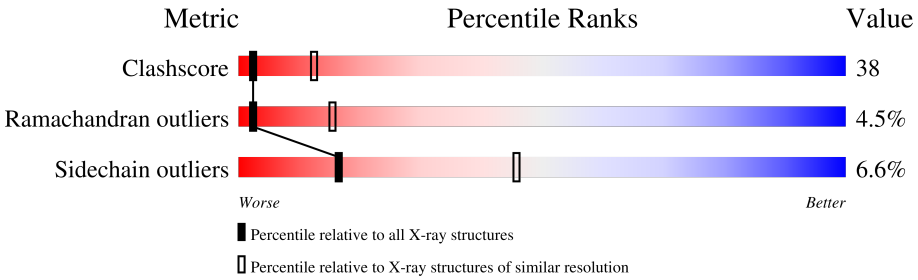
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.30 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))
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	602	68% 27%
1	M	602	25% 55% 15%
2	B	243	72% 26%
2	N	243	49% 42% 7%
3	C	130	62% 35%
3	O	130	53% 42% 5%
4	D	119	50% 47%
4	P	119	45% 49%

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	MQ7	D	700	-	-	X	-
6	FAD	M	803	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 17046 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4448	2775	802	840	31			
1	M	577	Total	C	N	O	S	0	0	0
			4448	2775	802	840	31			

- Molecule 2 is a protein called Fumarate reductase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			
2	N	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			

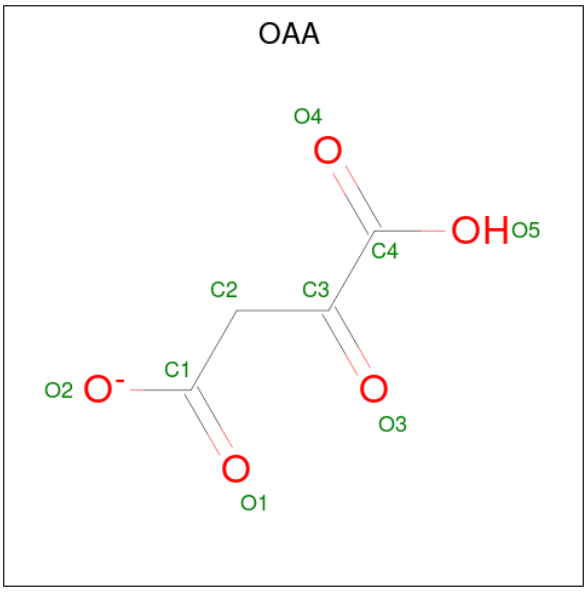
- Molecule 3 is a protein called Fumarate reductase 15 kDa hydrophobic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			
3	O	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			

- Molecule 4 is a protein called Fumarate reductase 13 kDa hydrophobic protein.

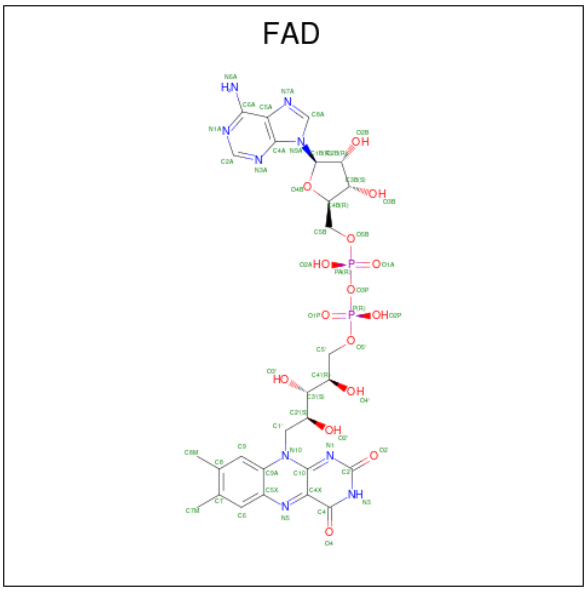
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 4 5	0	0
5	M	1	Total C O 9 4 5	0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

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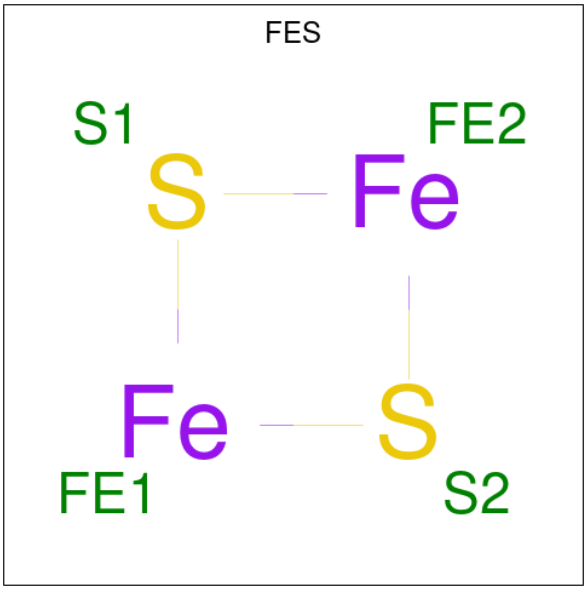
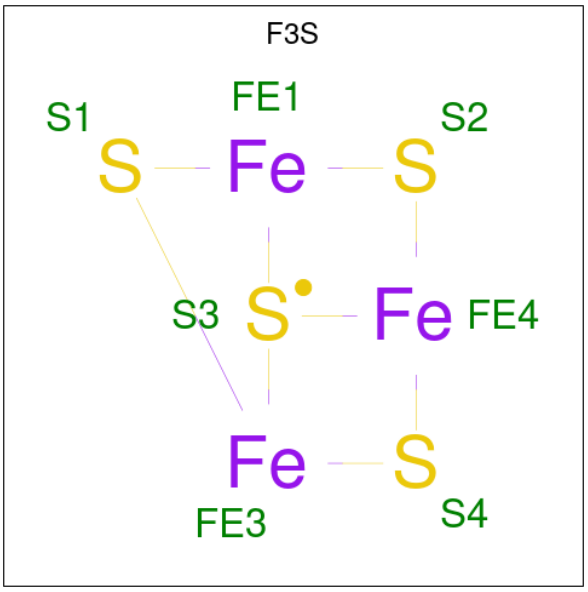
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



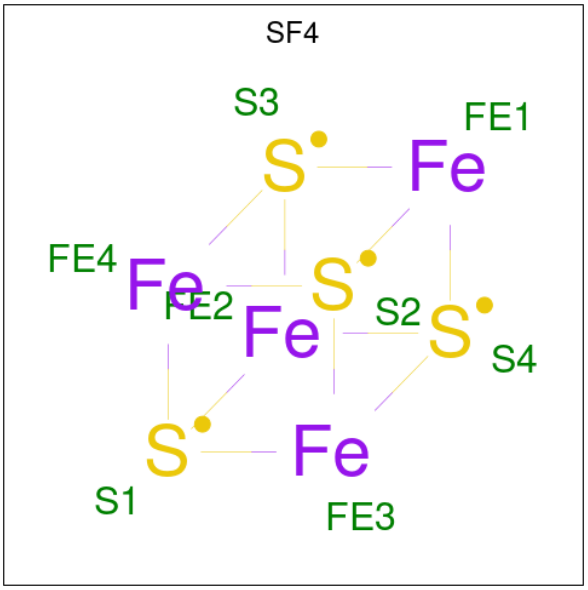
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	Fe	S		0	0
			4	2	2			
7	N	1	Total	Fe	S		0	0
			4	2	2			

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



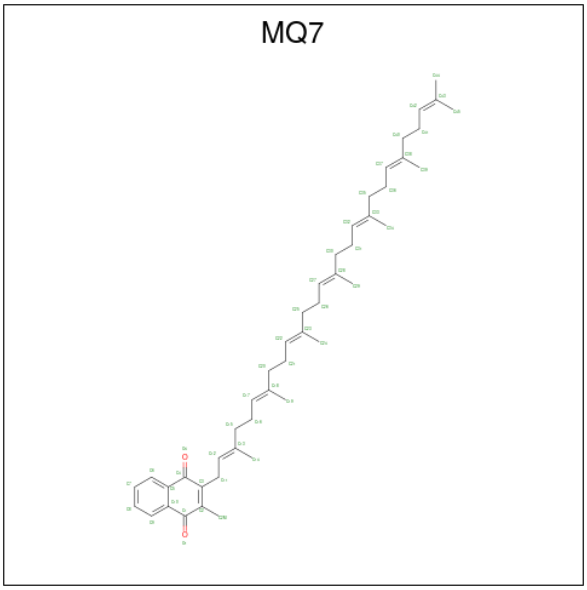
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Fe S 7 3 4	0	0
8	N	1	Total Fe S 7 3 4	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



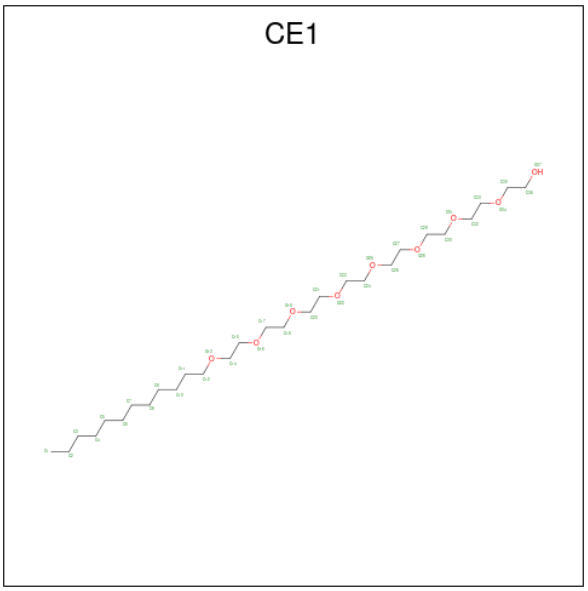
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 8 4 4	0	0
9	N	1	Total Fe S 8 4 4	0	0

- Molecule 10 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 24 22 2	0	0
10	D	1	Total C O 24 22 2	0	0
10	N	1	Total C O 24 22 2	0	0
10	P	1	Total C O 24 22 2	0	0

- Molecule 11 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: $C_{28}H_{58}O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total C O 37 28 9	0	0
11	D	1	Total C O 37 28 9	0	0
11	O	1	Total C O 37 28 9	0	0
11	O	1	Total C O 37 28 9	0	0

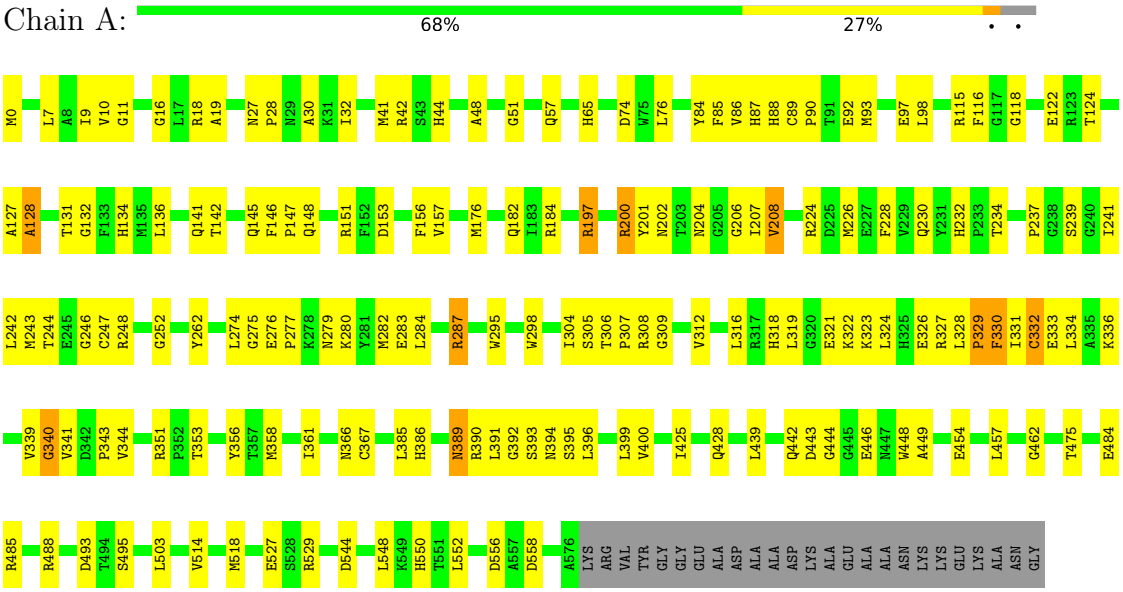
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

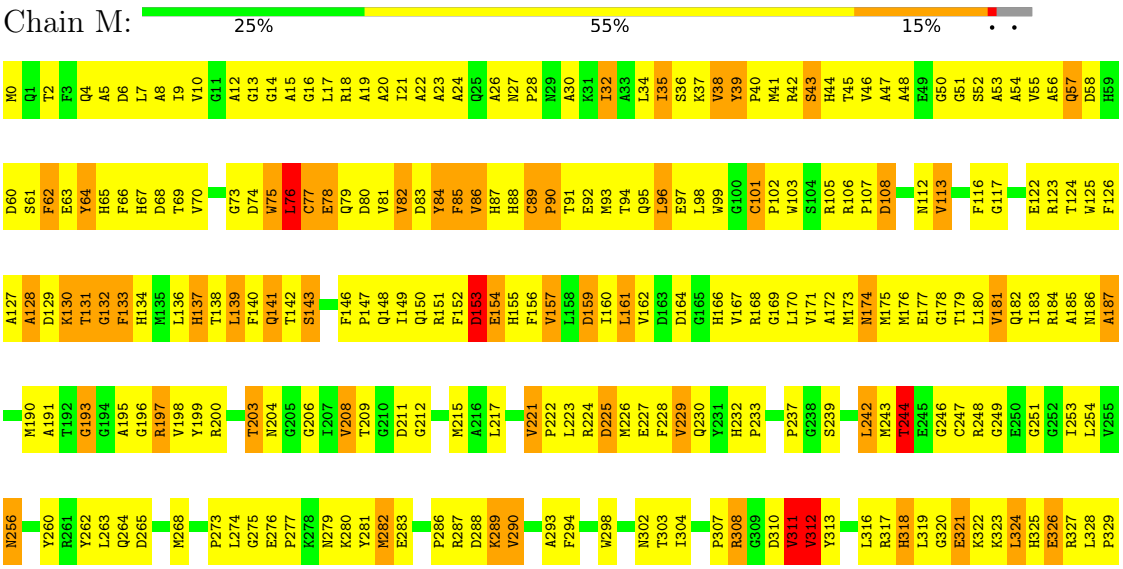
• Molecule 1: Fumarate reductase flavoprotein subunit

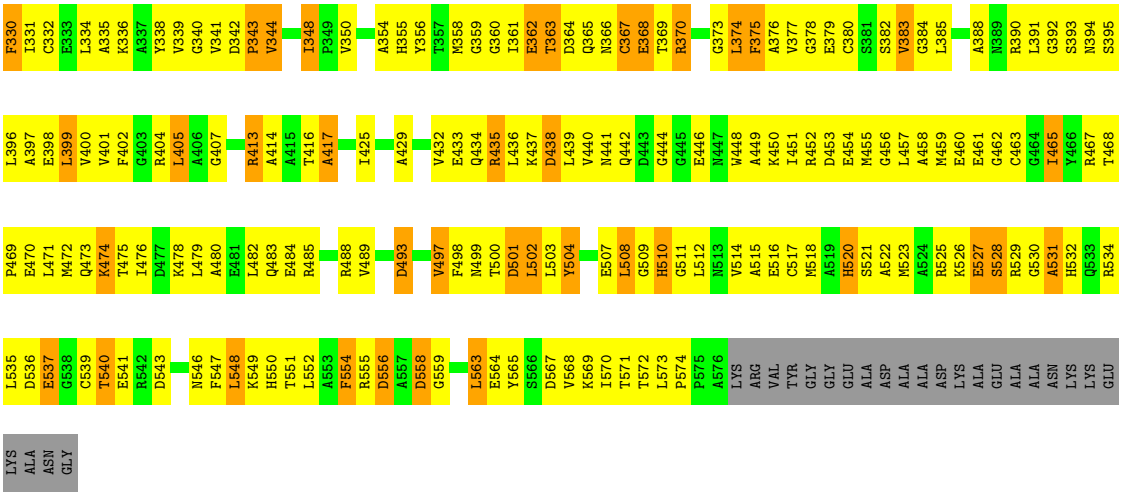
Chain A:



• Molecule 1: Fumarate reductase flavoprotein subunit

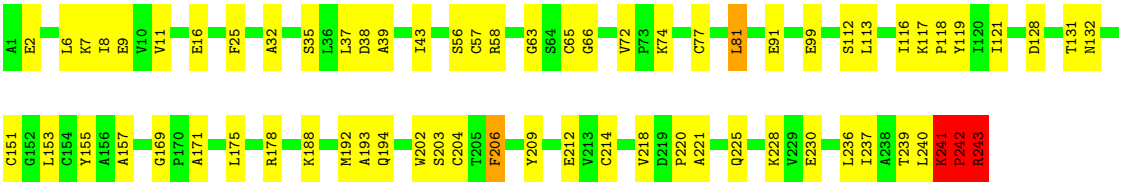
Chain M:





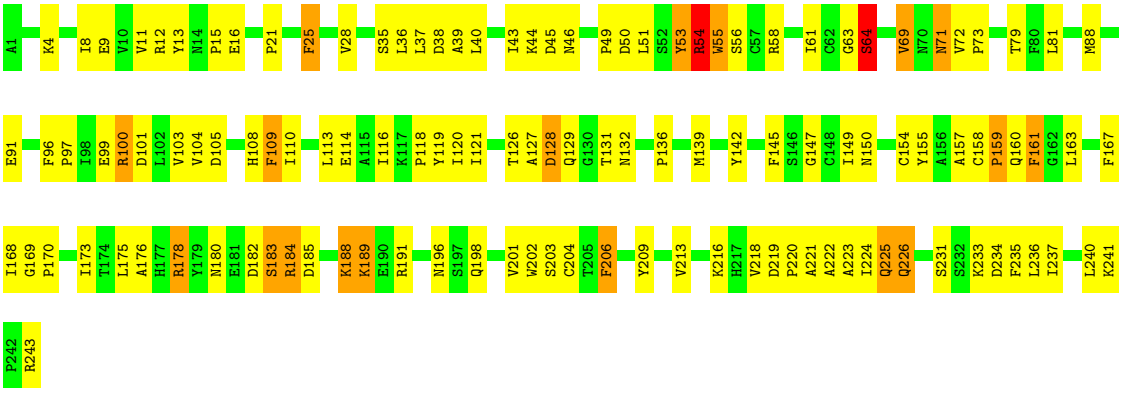
• Molecule 2: Fumarate reductase iron-sulfur protein

Chain B:



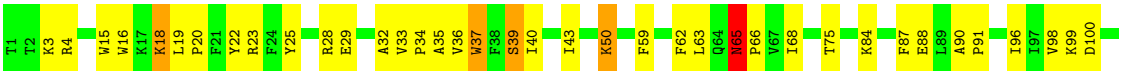
• Molecule 2: Fumarate reductase iron-sulfur protein

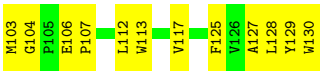
Chain N:



• Molecule 3: Fumarate reductase 15 kDa hydrophobic protein

Chain C:



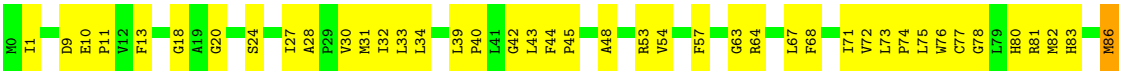


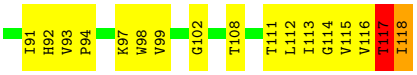
• Molecule 3: Fumarate reductase 15 kDa hydrophobic protein

Chain O:

• Molecule 4: Fumarate reductase 13 kDa hydrophobic protein

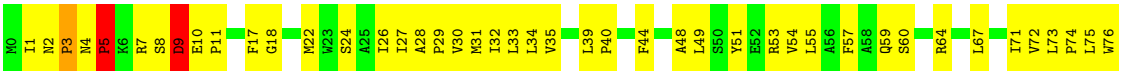
Chain D:





• Molecule 4: Fumarate reductase 13 kDa hydrophobic protein

Chain P:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.59Å 138.09Å 275.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17046	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, SF4, FES, MQ7, CE1, OAA, FAD

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	0.59	0/4540	0.80	2/6139 (0.0%)
1	M	0.48	0/4540	0.75	1/6139 (0.0%)
2	B	0.98	6/1931 (0.3%)	1.04	11/2617 (0.4%)
2	N	0.80	9/1931 (0.5%)	0.89	8/2617 (0.3%)
3	C	0.50	0/1094	0.69	1/1496 (0.1%)
3	O	0.52	0/1094	0.68	0/1496
4	D	0.53	0/956	0.74	0/1303
4	P	0.99	2/956 (0.2%)	0.78	1/1303 (0.1%)
All	All	0.66	17/17042 (0.1%)	0.81	24/23110 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	N	0	3
4	P	0	1
All	All	0	5

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	9	ASP	C-N	-21.89	0.83	1.34
2	B	243	ARG	CA-C	19.61	2.04	1.52
2	B	243	ARG	C-O	17.19	1.56	1.23
4	P	95	ALA	C-N	13.40	1.57	1.33
2	N	69	VAL	C-N	-13.14	1.03	1.34

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	243	ARG	CB-CG-CD	16.45	154.36	111.60
2	B	243	ARG	NE-CZ-NH1	-11.92	114.34	120.30
2	N	54	ARG	O-C-N	-11.67	104.03	122.70
2	B	242	PRO	CA-N-CD	-11.40	95.53	111.50
2	B	243	ARG	NE-CZ-NH2	11.02	125.81	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	243	ARG	Sidechain
2	N	183	SER	Mainchain
2	N	54	ARG	Mainchain
2	N	64	SER	Mainchain
4	P	9	ASP	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4448	0	4335	143	0
1	M	4448	0	4333	662	0
2	B	1888	0	1837	72	0
2	N	1888	0	1833	172	0
3	C	1058	0	1108	52	0
3	O	1058	0	1108	82	0
4	D	926	0	971	90	0
4	P	926	0	970	106	0
5	A	9	0	2	1	0
5	M	9	0	2	1	0
6	A	53	0	31	8	0
6	M	53	0	31	24	0
7	B	4	0	0	1	0
7	N	4	0	0	0	0
8	B	7	0	0	0	0
8	N	7	0	0	1	0
9	B	8	0	0	0	0
9	N	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	24	0	23	4	0
10	D	24	0	23	26	0
10	N	24	0	23	14	0
10	P	24	0	23	20	0
11	D	74	0	116	8	0
11	O	74	0	116	1	0
All	All	17046	0	16885	1285	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 38.

The worst 5 of 1285 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:44:HIS:NE2	6:A:703:FAD:HM82	1.16	1.45
1:M:98:LEU:CD2	2:N:132:ASN:HD21	1.28	1.42
1:M:44:HIS:NE2	6:M:803:FAD:HM82	1.06	1.32
1:M:493:ASP:OD2	2:N:50:ASP:HA	1.27	1.31
1:M:98:LEU:HD23	2:N:132:ASN:ND2	1.42	1.31

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	575/602 (96%)	529 (92%)	37 (6%)	9 (2%)	9 36
1	M	575/602 (96%)	355 (62%)	153 (27%)	67 (12%)	0 2
2	B	241/243 (99%)	215 (89%)	22 (9%)	4 (2%)	9 35
2	N	241/243 (99%)	205 (85%)	34 (14%)	2 (1%)	19 51
3	C	128/130 (98%)	121 (94%)	5 (4%)	2 (2%)	9 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	O	128/130 (98%)	113 (88%)	12 (9%)	3 (2%)	6 29
4	D	117/119 (98%)	101 (86%)	13 (11%)	3 (3%)	5 27
4	P	117/119 (98%)	99 (85%)	12 (10%)	6 (5%)	2 13
All	All	2122/2188 (97%)	1738 (82%)	288 (14%)	96 (4%)	2 15

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	242	PRO
4	D	99	VAL
1	M	57	GLN
1	M	76	LEU
1	M	85	PHE

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	460/475 (97%)	448 (97%)	12 (3%)	46 71
1	M	460/475 (97%)	400 (87%)	60 (13%)	4 17
2	B	205/205 (100%)	197 (96%)	8 (4%)	32 62
2	N	205/205 (100%)	191 (93%)	14 (7%)	16 44
3	C	111/111 (100%)	104 (94%)	7 (6%)	18 47
3	O	111/111 (100%)	103 (93%)	8 (7%)	14 41
4	D	97/97 (100%)	94 (97%)	3 (3%)	40 67
4	P	97/97 (100%)	93 (96%)	4 (4%)	30 61
All	All	1746/1776 (98%)	1630 (93%)	116 (7%)	16 46

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	225	ASP

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Mol	Chain	Res	Type
3	O	65	ASN
1	M	363	THR
3	O	61	ASP
2	N	189	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	264	GLN
1	M	409	GLN
4	P	4	ASN
1	M	279	ASN
1	M	325	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	FAD	M	803	1	53,58,58	1.55	10 (18%)	68,89,89	1.43	10 (14%)
10	MQ7	N	801	-	25,25,49	3.47	6 (24%)	31,34,63	2.48	9 (29%)
5	OAA	M	802	-	8,8,8	1.22	1 (12%)	9,10,10	1.17	1 (11%)
9	SF4	B	246	2	0,12,12	-	-	-		
5	OAA	A	702	-	8,8,8	1.14	0	9,10,10	1.01	1 (11%)
11	CE1	D	710	-	36,36,36	1.00	0	35,35,35	1.67	14 (40%)
10	MQ7	B	701	-	25,25,49	3.27	6 (24%)	31,34,63	2.32	8 (25%)
6	FAD	A	703	1	53,58,58	1.66	12 (22%)	68,89,89	1.64	14 (20%)
8	F3S	N	245	2	0,9,9	-	-	-		
10	MQ7	D	700	-	25,25,49	3.29	5 (20%)	31,34,63	2.32	10 (32%)
9	SF4	N	246	2	0,12,12	-	-	-		
10	MQ7	P	800	-	25,25,49	3.23	5 (20%)	31,34,63	2.31	11 (35%)
11	CE1	O	811	-	36,36,36	1.23	4 (11%)	35,35,35	1.82	13 (37%)
11	CE1	O	812	-	36,36,36	1.12	0	35,35,35	1.57	7 (20%)
8	F3S	B	245	2	0,9,9	-	-	-		
11	CE1	D	810	-	36,36,36	1.10	0	35,35,35	1.70	15 (42%)
7	FES	N	244	2	0,4,4	-	-	-		
7	FES	B	244	2	0,4,4	-	-	-		

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
6	FAD	M	803	1	-	10/30/50/50	0/6/6/6
10	MQ7	N	801	-	-	3/13/33/61	0/2/2/2
5	OAA	M	802	-	-	6/8/8/8	-
9	SF4	B	246	2	-	-	0/6/5/5
5	OAA	A	702	-	-	6/8/8/8	-
11	CE1	D	710	-	-	16/34/34/34	-
10	MQ7	B	701	-	-	3/13/33/61	0/2/2/2
6	FAD	A	703	1	-	8/30/50/50	0/6/6/6
8	F3S	N	245	2	-	-	0/3/3/3
10	MQ7	D	700	-	-	2/13/33/61	0/2/2/2
10	MQ7	P	800	-	-	1/13/33/61	0/2/2/2
11	CE1	O	811	-	-	15/34/34/34	-
11	CE1	O	812	-	-	18/34/34/34	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	N	246	2	-	-	0/6/5/5
8	F3S	B	245	2	-	-	0/3/3/3
11	CE1	D	810	-	-	16/34/34/34	-
7	FES	N	244	2	-	-	0/1/1/1
7	FES	B	244	2	-	-	0/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	801	MQ7	C11-C12	-11.95	1.33	1.50
10	D	700	MQ7	C11-C12	-11.04	1.34	1.50
10	P	800	MQ7	C11-C12	-10.87	1.34	1.50
10	B	701	MQ7	C11-C12	-10.24	1.35	1.50
10	N	801	MQ7	C12-C13	9.78	1.56	1.33

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	N	801	MQ7	C11-C3-C4	-7.64	110.33	118.50
10	D	700	MQ7	C11-C3-C4	-7.39	110.59	118.50
10	B	701	MQ7	C11-C3-C4	-7.37	110.61	118.50
10	P	800	MQ7	C11-C3-C4	-7.02	110.99	118.50
10	P	800	MQ7	C12-C11-C3	6.17	128.69	112.05

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	OAA	C1-C2-C3-C4
5	A	702	OAA	O3-C3-C4-O4
5	A	702	OAA	O3-C3-C4-O5
5	A	702	OAA	C2-C3-C4-O4
5	A	702	OAA	C2-C3-C4-O5

There are no ring outliers.

13 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	803	FAD	24	0
10	N	801	MQ7	14	0
5	M	802	OAA	1	0

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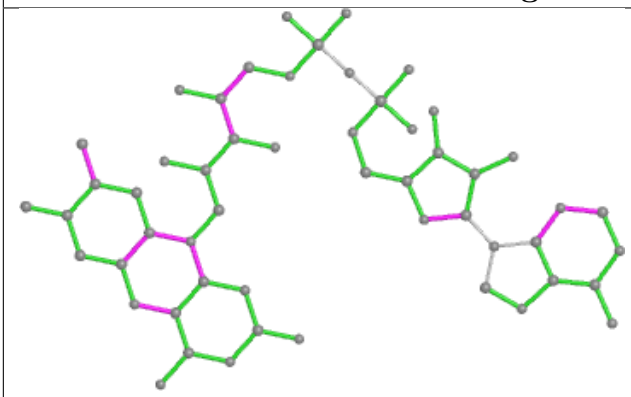
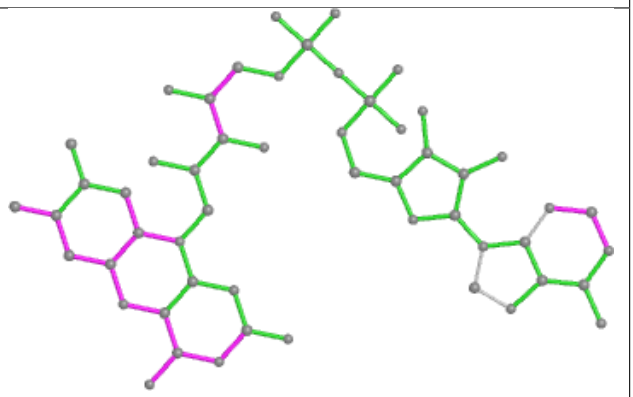
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	OAA	1	0
11	D	710	CE1	3	0
10	B	701	MQ7	4	0
6	A	703	FAD	8	0
8	N	245	F3S	1	0
10	D	700	MQ7	26	0
10	P	800	MQ7	20	0
11	O	812	CE1	1	0
11	D	810	CE1	5	0
7	B	244	FES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

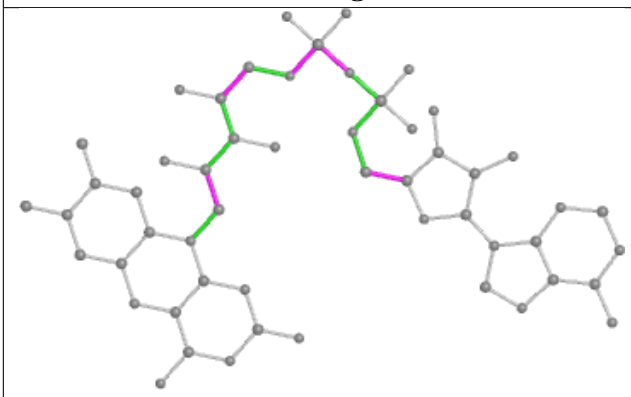
Ligand FAD M 803



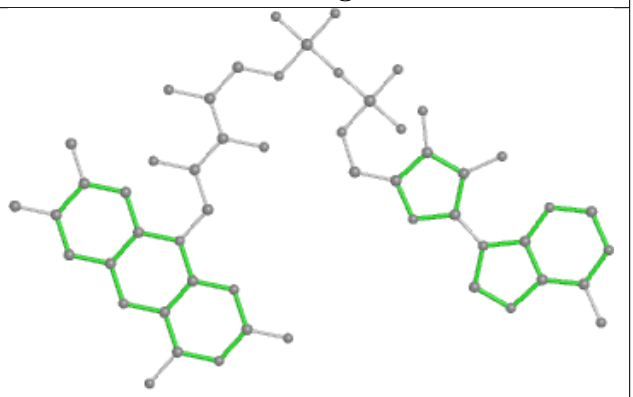
Bond lengths



Bond angles

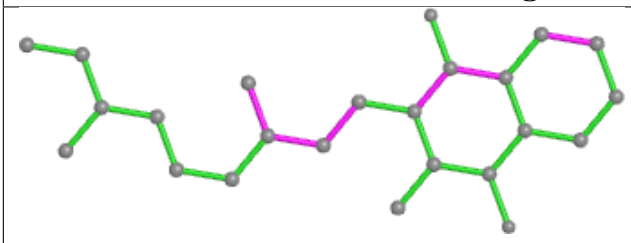


Torsions



Rings

Ligand MQ7 N 801



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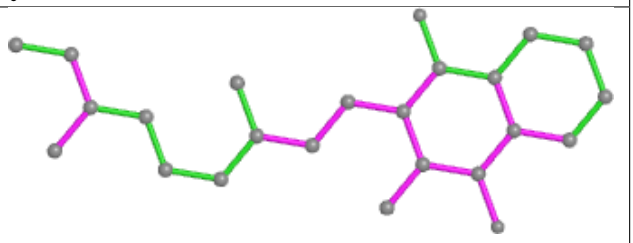
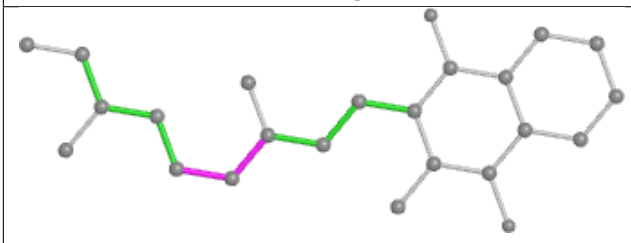
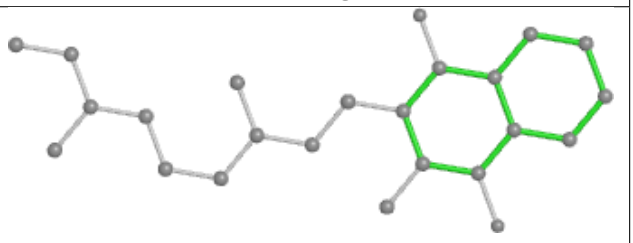


Bond angles

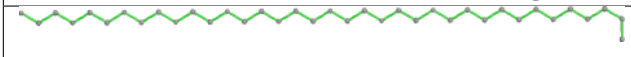


Torsions

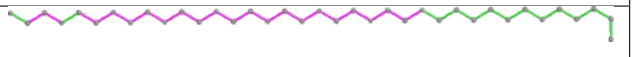


Rings

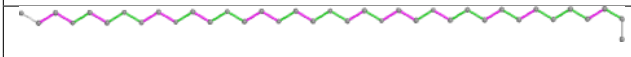
Ligand CE1 D 710



Bond lengths



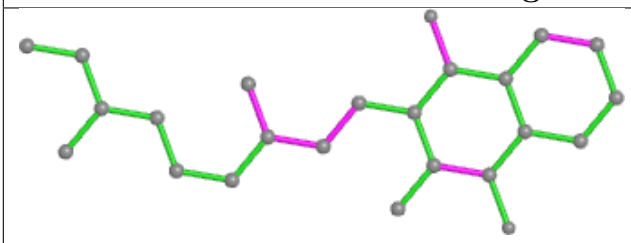
Bond angles



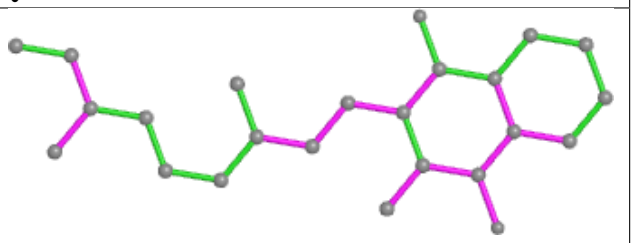
Torsions

Rings

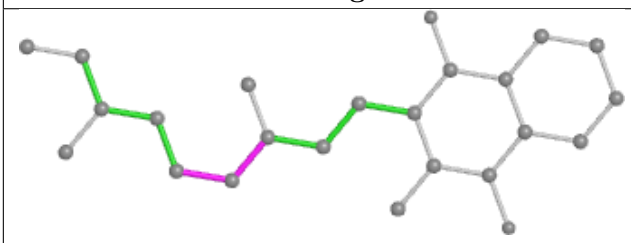
Ligand MQ7 B 701



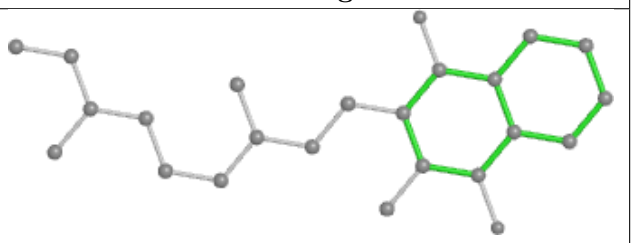
Bond lengths



Bond angles

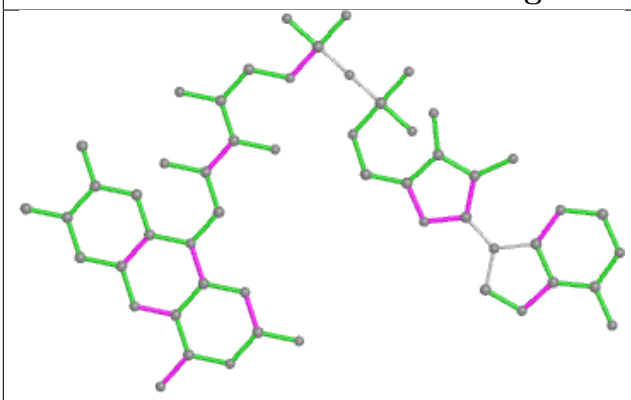


Torsions

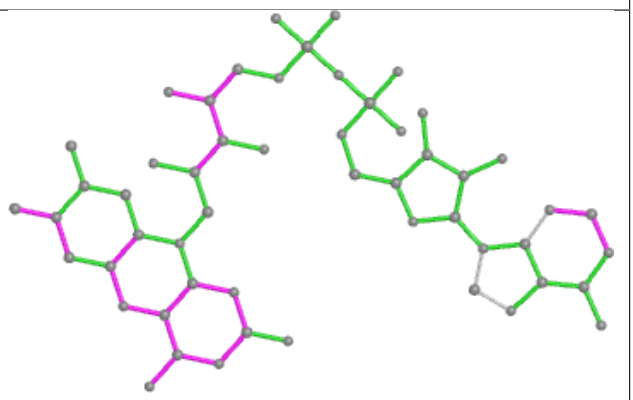


Rings

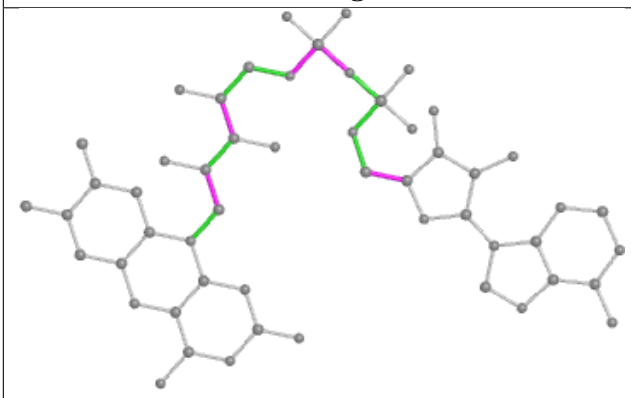
Ligand FAD A 703



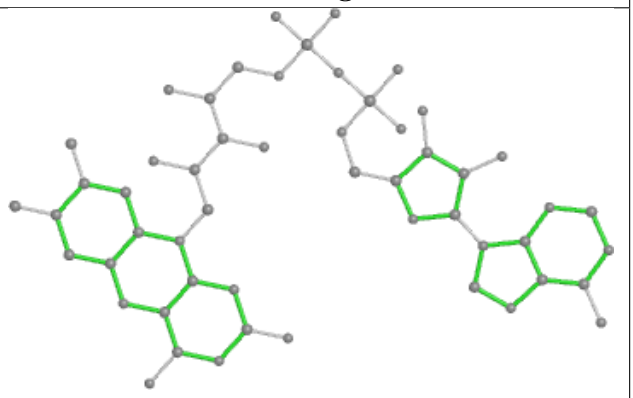
Bond lengths



Bond angles

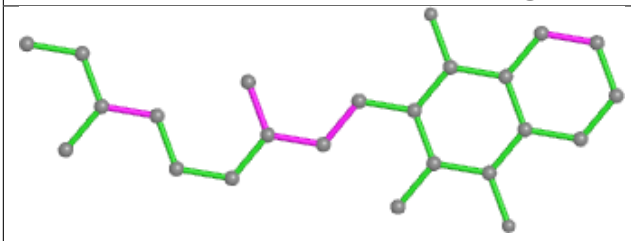


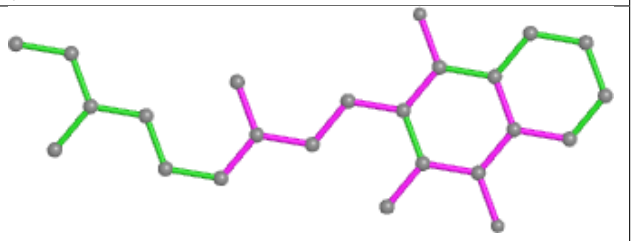
Torsions

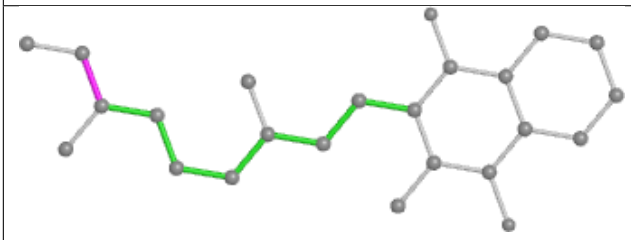


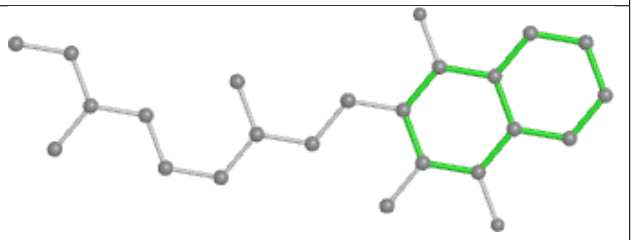
Rings

Ligand MQ7 D 700

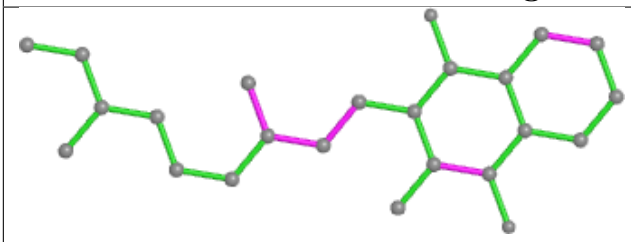

Bond lengths

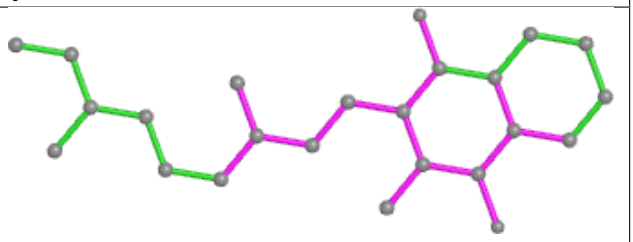

Bond angles

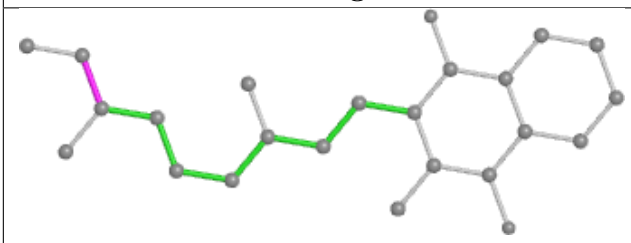

Torsions

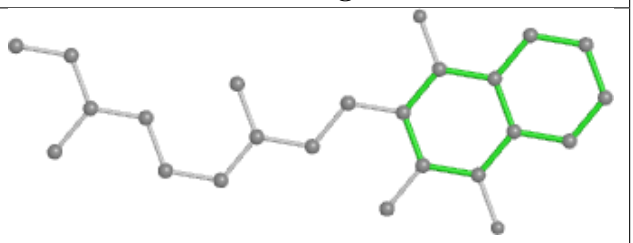

Rings

Ligand MQ7 P 800

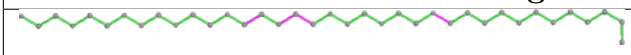

Bond lengths


Bond angles


Torsions


Rings

Ligand CE1 O 811

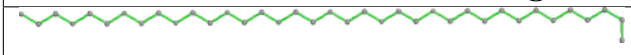

Bond lengths

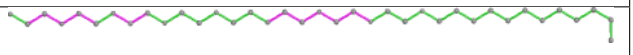

Bond angles

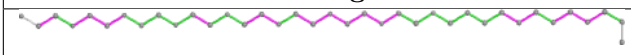

Torsions


Rings

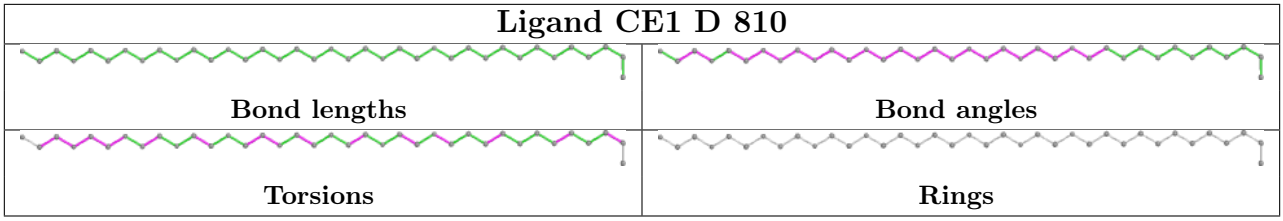
Ligand CE1 O 812


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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	N	3
4	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	4:LYS	C	5:ASN	N	1.14
1	N	159:PRO	C	160:GLN	N	1.04
1	N	69:VAL	C	70:ASN	N	1.03
1	P	9:ASP	C	10:GLU	N	0.83

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.