



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 12:47 PM UTC

PDB ID : 1KF6 / pdb_00001kf6
Title : E. coli Quinol-Fumarate Reductase with Bound Inhibitor HQNO
Authors : Iverson, T.M.; Luna-Chavez, C.; Croal, L.R.; Cecchini, G.; Rees, D.C.
Deposited on : 2001-11-19
Resolution : 2.70 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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

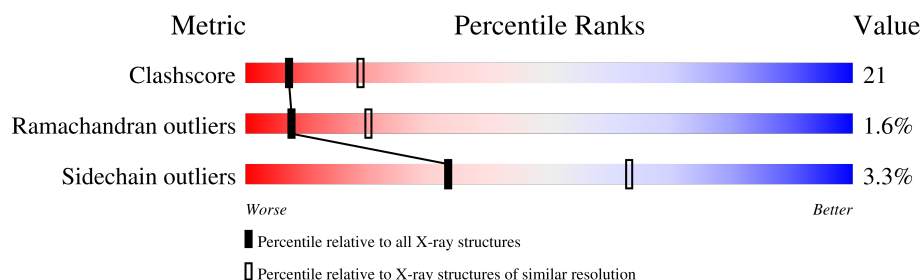
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	602	
1	M	602	
2	B	243	
2	N	243	
3	C	130	
3	O	130	
4	D	119	
4	P	119	

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
12	SF4	N	246	-	-	X	-
7	ACT	N	803	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 17071 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.

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			

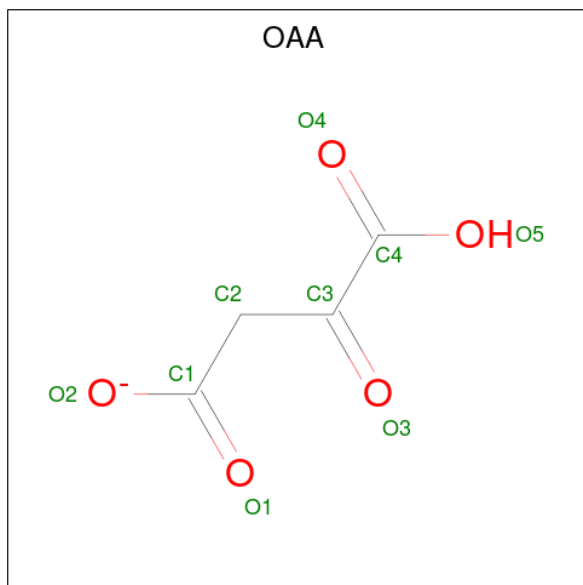
- Molecule 4 is a protein called FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN.

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 POTASSIUM ION (CCD ID: K) (formula: K).

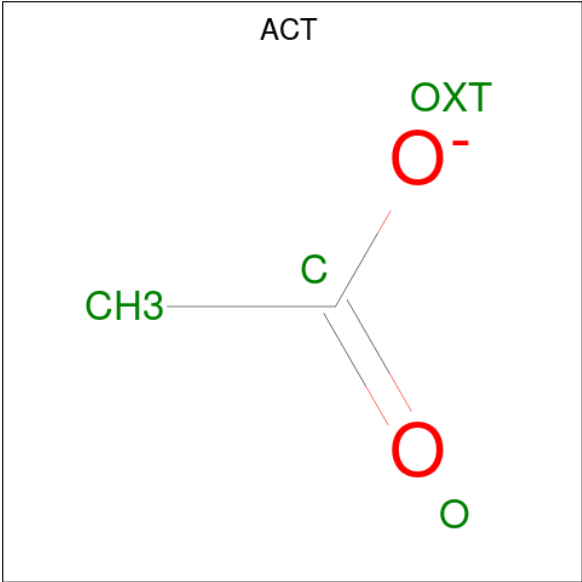
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	M	1	Total K 1 1	0	0

- Molecule 6 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$).



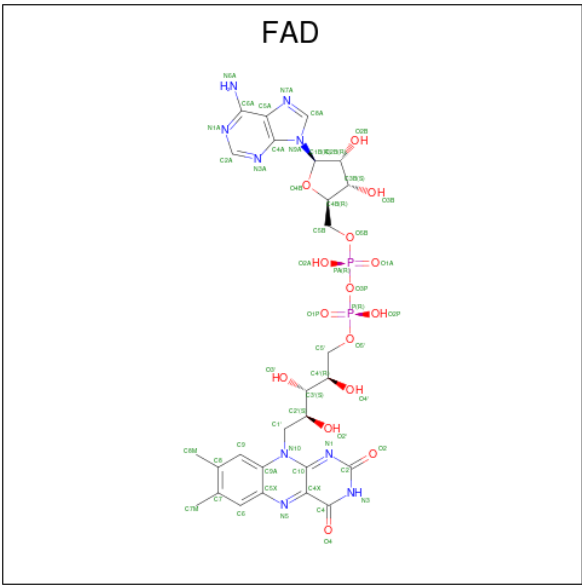
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 4 5	0	0
6	M	1	Total C O 9 4 5	0	0

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O		0	0
			4	2	2			
7	B	1	Total	C	O		0	0
			4	2	2			
7	N	1	Total	C	O		0	0
			4	2	2			

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



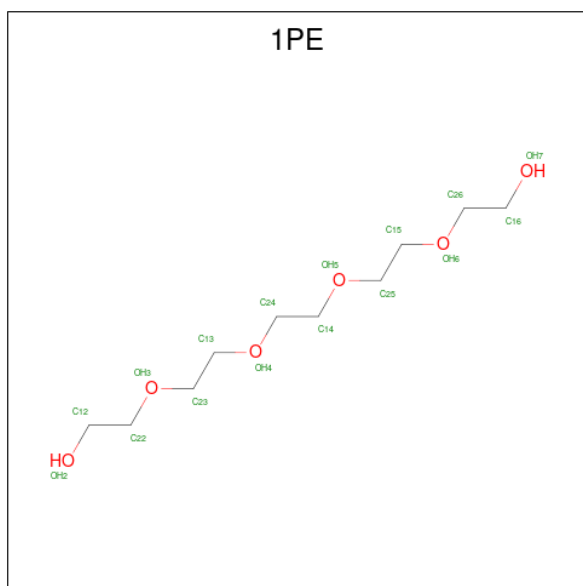
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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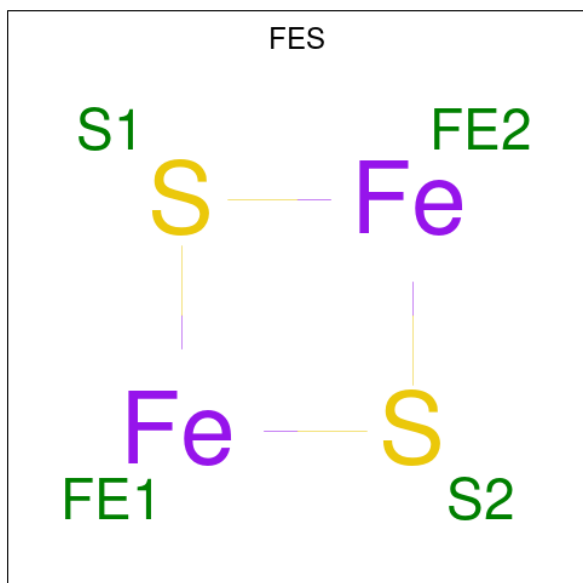
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 9 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



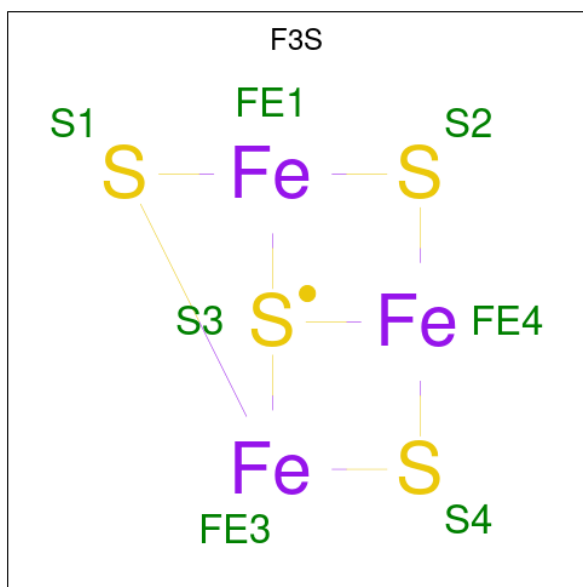
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



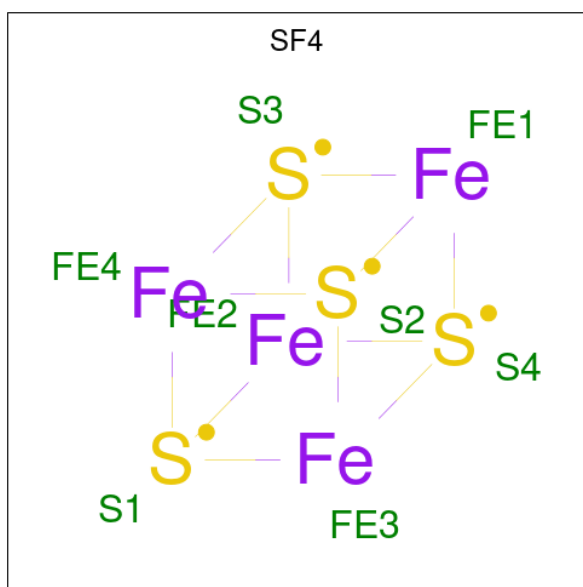
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			4	2	2		
10	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 11 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



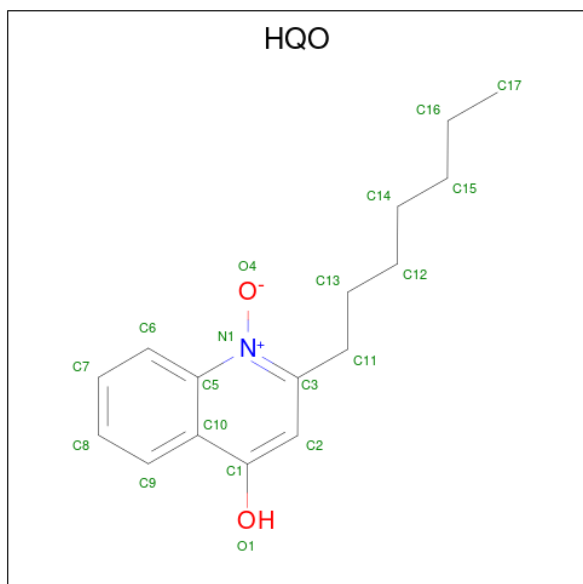
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			7	3	4		
11	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 12 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 13 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (CCD ID: HQO) (formula: $C_{16}H_{21}NO_2$).



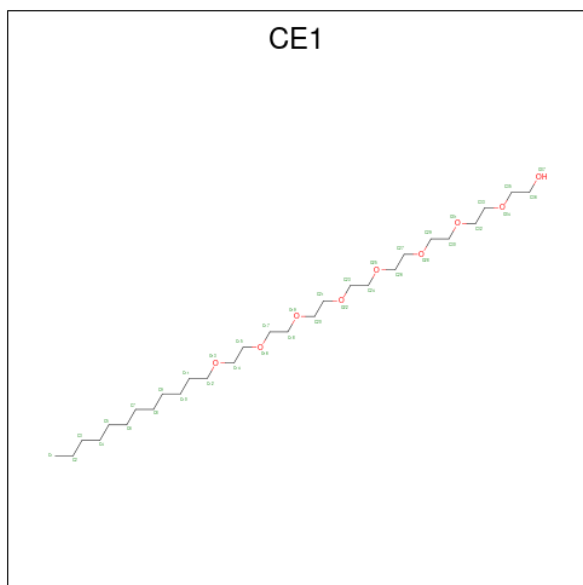
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			19	16	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	N	1	Total	C	N	O	0	0
			19	16	1	2		

- Molecule 14 is O-DODECANYL OCTAETHYLENE GLYCOL (CCD ID: CE1) (formula: $C_{28}H_{58}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	O	1	Total	C	O	0	0
			37	28	9		
14	O	1	Total	C	O	0	0
			37	28	9		
14	O	1	Total	C	O	0	0
			37	28	9		
14	P	1	Total	C	O	0	0
			37	28	9		
14	P	1	Total	C	O	0	0
			37	28	9		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	10	Total	O	0	0
			10	10		
15	B	1	Total	O	0	0
			1	1		
15	M	4	Total	O	0	0
			4	4		

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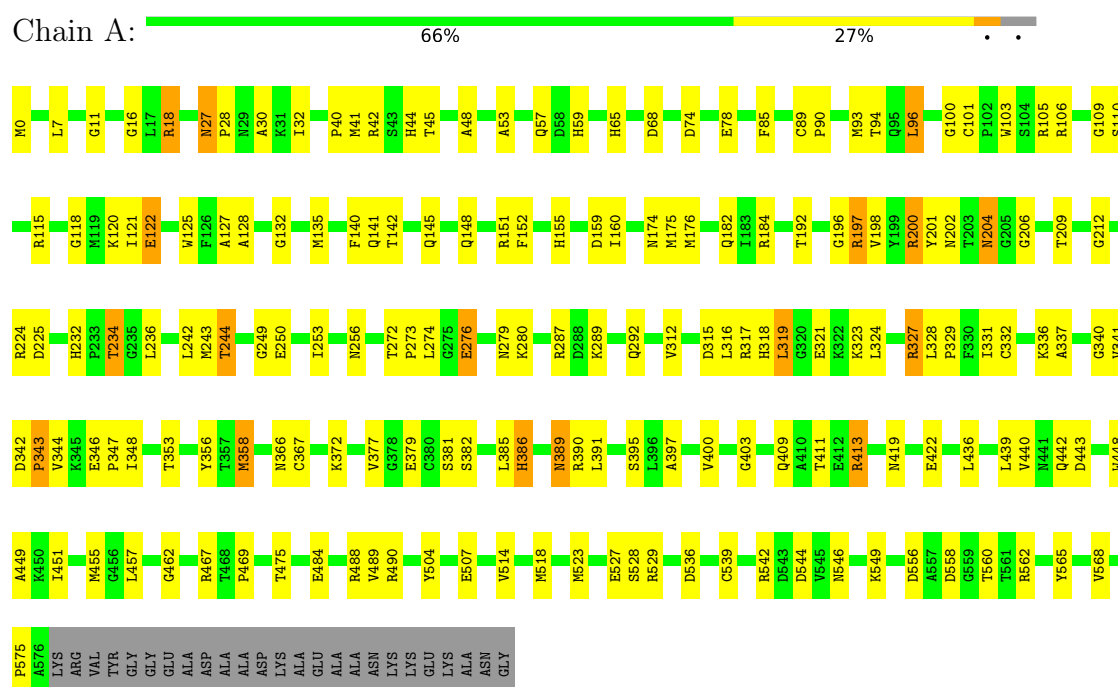
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	N	1	Total	O	0	0
			1	1		

3 Residue-property plots

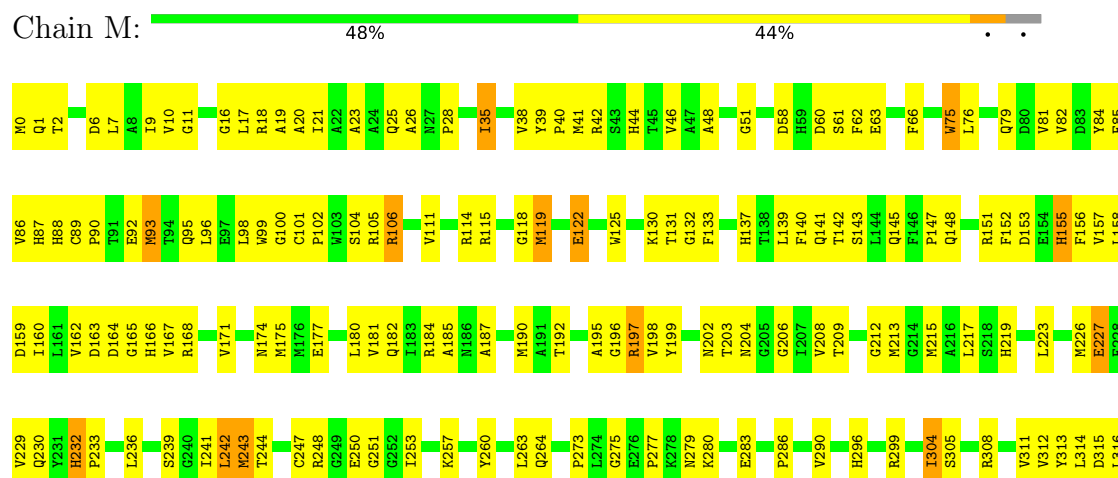
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

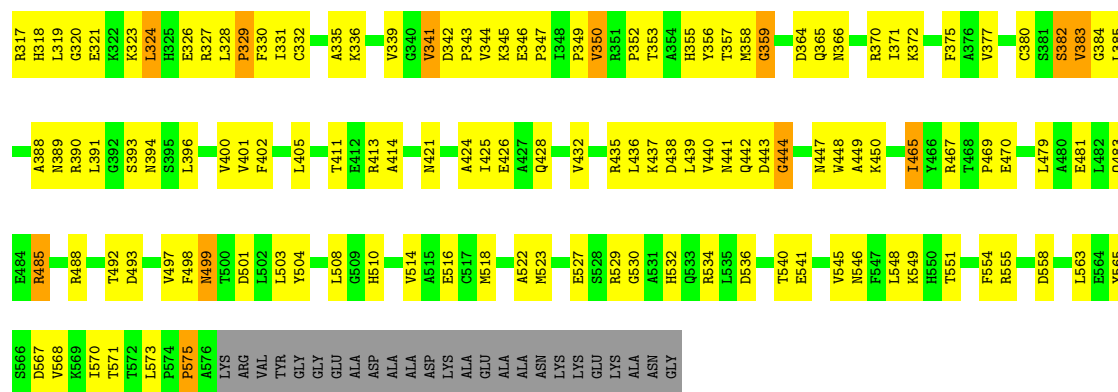
Note EDS was not executed.

• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN



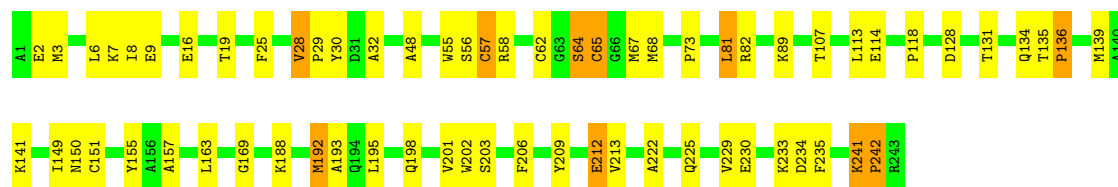
• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN





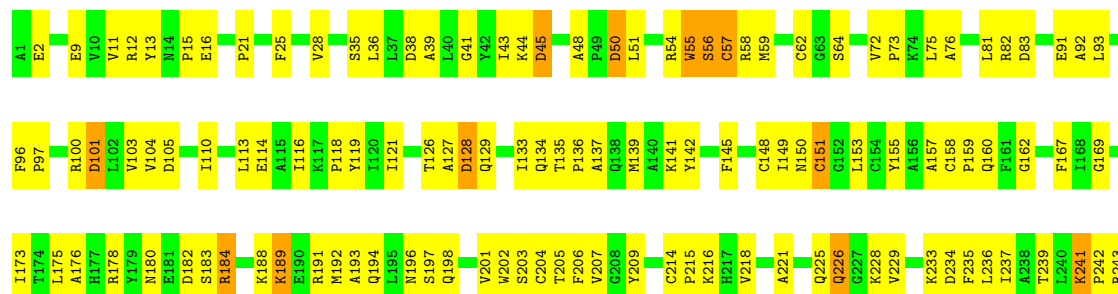
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain B: 73% 23%



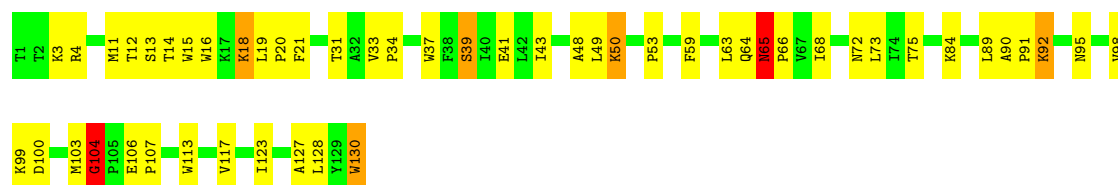
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain N: 50% 45% 5%



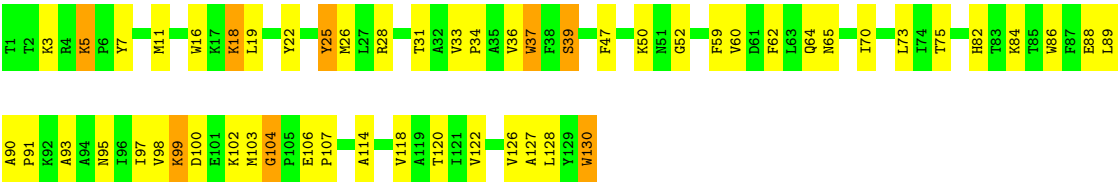
• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

Chain C: 61% 34%

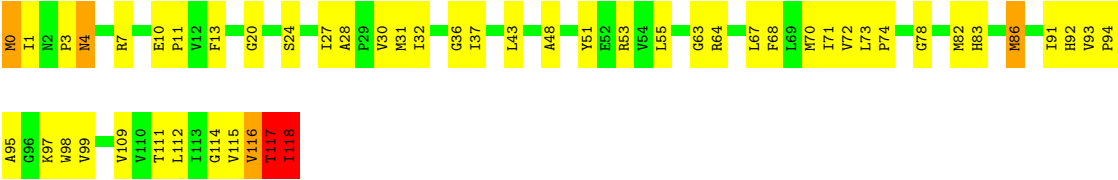


• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

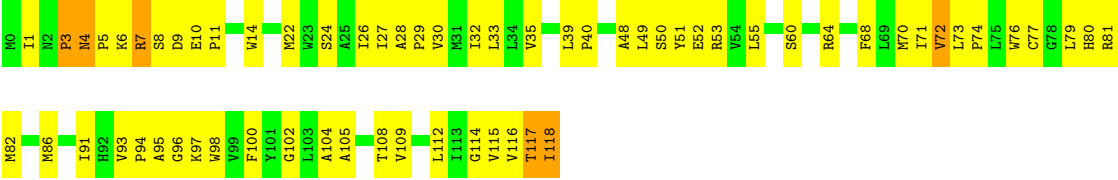
Chain O: 58% 35% 6%



• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN



• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN



4 Data and refinement statistics

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	96.50Å 137.84Å 273.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.231 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17071	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, K, SF4, FAD, FES, OAA, HQO, CE1, ACT, F3S

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	1.04	1/4540 (0.0%)	1.23	23/6139 (0.4%)
1	M	0.68	3/4540 (0.1%)	1.11	10/6139 (0.2%)
2	B	0.99	2/1931 (0.1%)	1.22	14/2617 (0.5%)
2	N	0.74	3/1931 (0.2%)	1.13	6/2617 (0.2%)
3	C	0.99	6/1094 (0.5%)	1.21	6/1496 (0.4%)
3	O	0.87	5/1094 (0.5%)	1.14	4/1496 (0.3%)
4	D	1.01	4/956 (0.4%)	1.24	4/1303 (0.3%)
4	P	0.91	4/956 (0.4%)	1.12	4/1303 (0.3%)
All	All	0.90	28/17042 (0.2%)	1.17	71/23110 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	117	THR	CA-C	-12.17	1.40	1.53
3	C	65	ASN	C-O	-11.70	1.09	1.24
4	D	118	ILE	C-OXT	10.96	1.45	1.23
3	O	65	ASN	C-O	-8.75	1.12	1.24
4	D	117	THR	CA-C	-8.45	1.41	1.52

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	116	VAL	N-CA-C	-11.52	101.43	112.83
2	B	65	CYS	N-CA-C	11.16	126.00	112.38
2	B	64	SER	CA-C-N	9.68	136.09	120.60
2	B	64	SER	C-N-CA	9.68	136.09	120.60
4	D	72	VAL	N-CA-C	7.78	118.36	110.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	65	ASN	Mainchain,Peptide

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	128	0
1	M	4448	0	4335	270	0
2	B	1888	0	1837	54	0
2	N	1888	0	1837	112	0
3	C	1058	0	1108	49	0
3	O	1058	0	1108	52	0
4	D	926	0	971	48	0
4	P	926	0	971	68	0
5	A	1	0	0	0	0
5	M	1	0	0	0	0
6	A	9	0	2	2	0
6	M	9	0	2	0	0
7	A	4	0	3	0	0
7	B	4	0	3	0	0
7	N	4	0	3	2	0
8	A	53	0	31	7	0
8	M	53	0	31	8	0
9	A	16	0	20	5	0
10	B	4	0	0	0	0
10	N	4	0	0	0	0
11	B	7	0	0	0	0
11	N	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	B	8	0	0	0	0
12	N	8	0	0	4	0
13	C	19	0	20	3	0
13	N	19	0	20	2	0
14	O	111	0	174	0	0
14	P	74	0	116	5	0
15	A	10	0	0	1	0
15	B	1	0	0	0	0
15	M	4	0	0	0	0
15	N	1	0	0	0	0
All	All	17071	0	16927	706	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 21.

The worst 5 of 706 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	8:A:721:FAD:C8M	1.89	1.33
1:M:44:HIS:NE2	8:M:821:FAD:HM82	1.02	1.33
1:M:44:HIS:NE2	8:M:821:FAD:C8M	1.98	1.27
1:A:44:HIS:NE2	8:A:721:FAD:HM82	0.93	1.24
1:M:421:ASN:HD22	1:M:424:ALA:HB2	1.17	1.04

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%)	541 (94%)	30 (5%)	4 (1%)	18 41
1	M	575/602 (96%)	487 (85%)	75 (13%)	13 (2%)	5 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	241/243 (99%)	224 (93%)	16 (7%)	1 (0%)	30	54
2	N	241/243 (99%)	215 (89%)	20 (8%)	6 (2%)	4	11
3	C	128/130 (98%)	120 (94%)	4 (3%)	4 (3%)	3	8
3	O	128/130 (98%)	114 (89%)	12 (9%)	2 (2%)	7	20
4	D	117/119 (98%)	111 (95%)	3 (3%)	3 (3%)	4	11
4	P	117/119 (98%)	102 (87%)	14 (12%)	1 (1%)	14	35
All	All	2122/2188 (97%)	1914 (90%)	174 (8%)	34 (2%)	7	20

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	18	LYS
3	C	65	ASN
1	M	244	THR
1	M	382	SER
1	A	318	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	460/475 (97%)	445 (97%)	15 (3%)	33	63
1	M	460/475 (97%)	441 (96%)	19 (4%)	27	56
2	B	205/205 (100%)	200 (98%)	5 (2%)	43	72
2	N	205/205 (100%)	199 (97%)	6 (3%)	37	67
3	C	111/111 (100%)	106 (96%)	5 (4%)	24	52
3	O	111/111 (100%)	108 (97%)	3 (3%)	39	69
4	D	97/97 (100%)	93 (96%)	4 (4%)	27	56
4	P	97/97 (100%)	96 (99%)	1 (1%)	68	86
All	All	1746/1776 (98%)	1688 (97%)	58 (3%)	33	63

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	118	ILE
3	O	37	TRP
1	M	164	ASP
3	O	5	LYS
2	N	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	186	ASN
1	M	441	ASN
3	O	72	ASN
1	M	204	ASN
1	M	409	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	CE1	O	813	-	36,36,36	1.21	0	35,35,35	1.94	15 (42%)
10	FES	N	244	2	0,4,4	-	-	-		
8	FAD	M	821	-	58,58,58	1.56	7 (12%)	85,89,89	1.58	15 (17%)
7	ACT	N	803	-	3,3,3	1.21	0	3,3,3	1.05	0
7	ACT	B	704	-	3,3,3	0.81	0	3,3,3	0.98	0
12	SF4	B	246	2	0,12,12	-	-	-		
14	CE1	O	811	-	36,36,36	1.14	0	35,35,35	1.95	16 (45%)
12	SF4	N	246	2	0,12,12	-	-	-		
6	OAA	M	802	-	8,8,8	1.29	1 (12%)	8,10,10	1.60	1 (12%)
6	OAA	A	702	-	8,8,8	1.30	1 (12%)	8,10,10	1.59	1 (12%)
8	FAD	A	721	-	58,58,58	1.81	14 (24%)	85,89,89	1.59	18 (21%)
9	1PE	A	705	-	15,15,15	1.65	0	14,14,14	2.27	9 (64%)
11	F3S	N	245	2	0,9,9	-	-	-		
7	ACT	A	703	-	3,3,3	0.97	0	3,3,3	1.32	0
14	CE1	O	812	-	36,36,36	1.14	0	35,35,35	1.88	15 (42%)
10	FES	B	244	2	0,4,4	-	-	-		
13	HQO	C	700	-	19,20,20	3.55	8 (42%)	20,26,26	1.09	2 (10%)
14	CE1	P	710	-	36,36,36	1.14	0	35,35,35	1.89	15 (42%)
13	HQO	N	800	-	19,20,20	3.55	8 (42%)	20,26,26	1.09	2 (10%)
14	CE1	P	810	-	36,36,36	1.14	0	35,35,35	1.98	15 (42%)
11	F3S	B	245	2	0,9,9	-	-	-		

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
8	FAD	A	721	-	-	6/34/50/50	0/6/6/6
9	1PE	A	705	-	-	6/13/13/13	-
14	CE1	O	812	-	-	17/34/34/34	-
11	F3S	N	245	2	-	-	0/3/3/3
12	SF4	B	246	2	-	-	0/6/5/5
10	FES	B	244	2	-	-	0/1/1/1
14	CE1	O	811	-	-	16/34/34/34	-
14	CE1	O	813	-	-	13/34/34/34	-
12	SF4	N	246	2	-	-	0/6/5/5
13	HQO	C	700	-	-	3/7/7/7	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CE1	P	710	-	-	16/34/34/34	-
13	HQO	N	800	-	-	3/7/7/7	0/2/2/2
14	CE1	P	810	-	-	15/34/34/34	-
10	FES	N	244	2	-	-	0/1/1/1
8	FAD	M	821	-	-	6/34/50/50	0/6/6/6
11	F3S	B	245	2	-	-	0/3/3/3
6	OAA	M	802	-	-	4/8/8/8	-
6	OAA	A	702	-	-	4/8/8/8	-

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	800	HQO	O4-N1	-13.29	1.23	1.38
13	C	700	HQO	O4-N1	-13.29	1.23	1.38
8	A	721	FAD	P-O3P	-5.22	1.53	1.59
8	A	721	FAD	PA-O3P	-4.84	1.54	1.59
8	M	821	FAD	P-O3P	-4.46	1.54	1.59

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	821	FAD	N3A-C2A-N1A	-5.84	119.73	128.58
14	P	810	CE1	O28-C27-C26	4.60	131.30	110.35
8	A	721	FAD	C5A-C4A-N3A	-4.10	121.06	126.72
8	A	721	FAD	N3A-C4A-N9A	4.10	134.14	127.17
8	M	821	FAD	C4-N3-C2	-4.07	118.42	125.64

There are no chirality outliers.

5 of 109 torsion outliers are listed below:

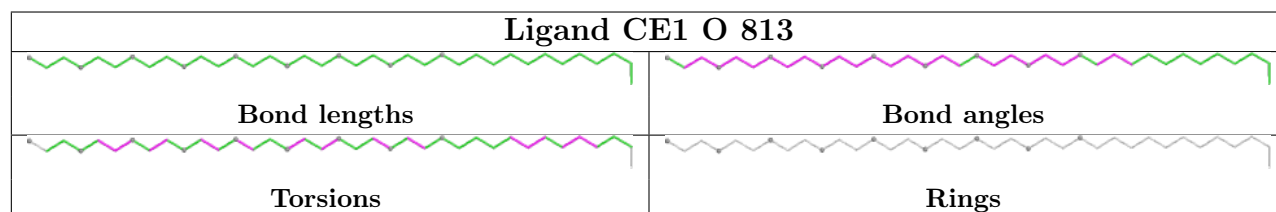
Mol	Chain	Res	Type	Atoms
6	A	702	OAA	O3-C3-C4-O4
6	A	702	OAA	O3-C3-C4-O5
6	A	702	OAA	C2-C3-C4-O5
6	M	802	OAA	O3-C3-C4-O4
6	M	802	OAA	O3-C3-C4-O5

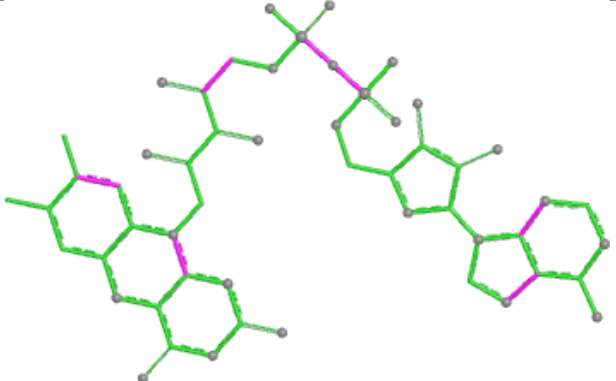
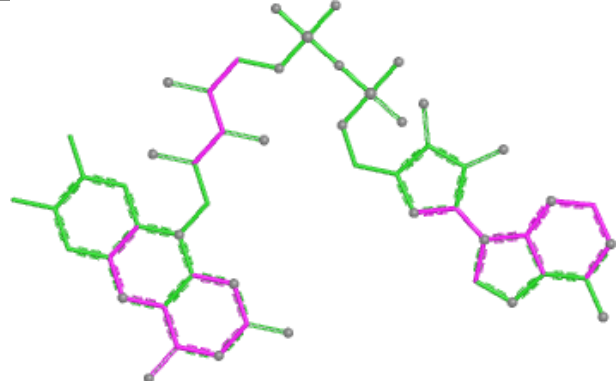
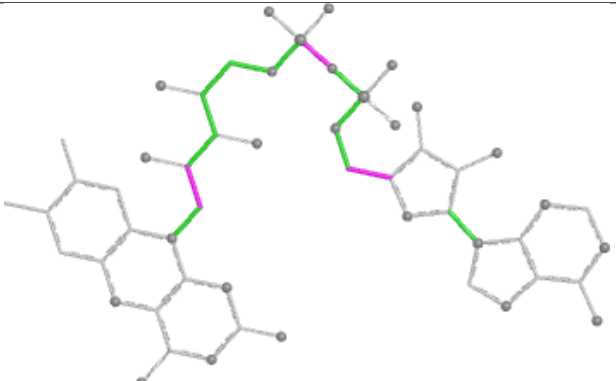
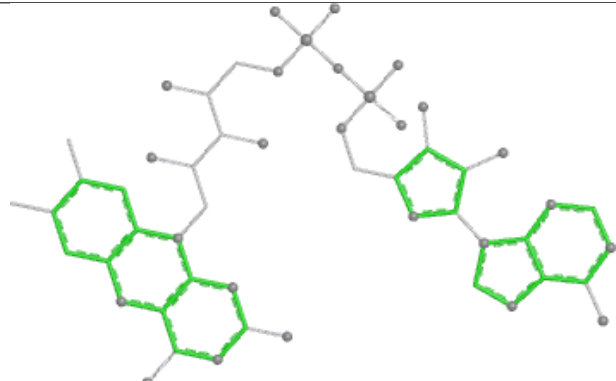
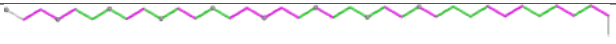
There are no ring outliers.

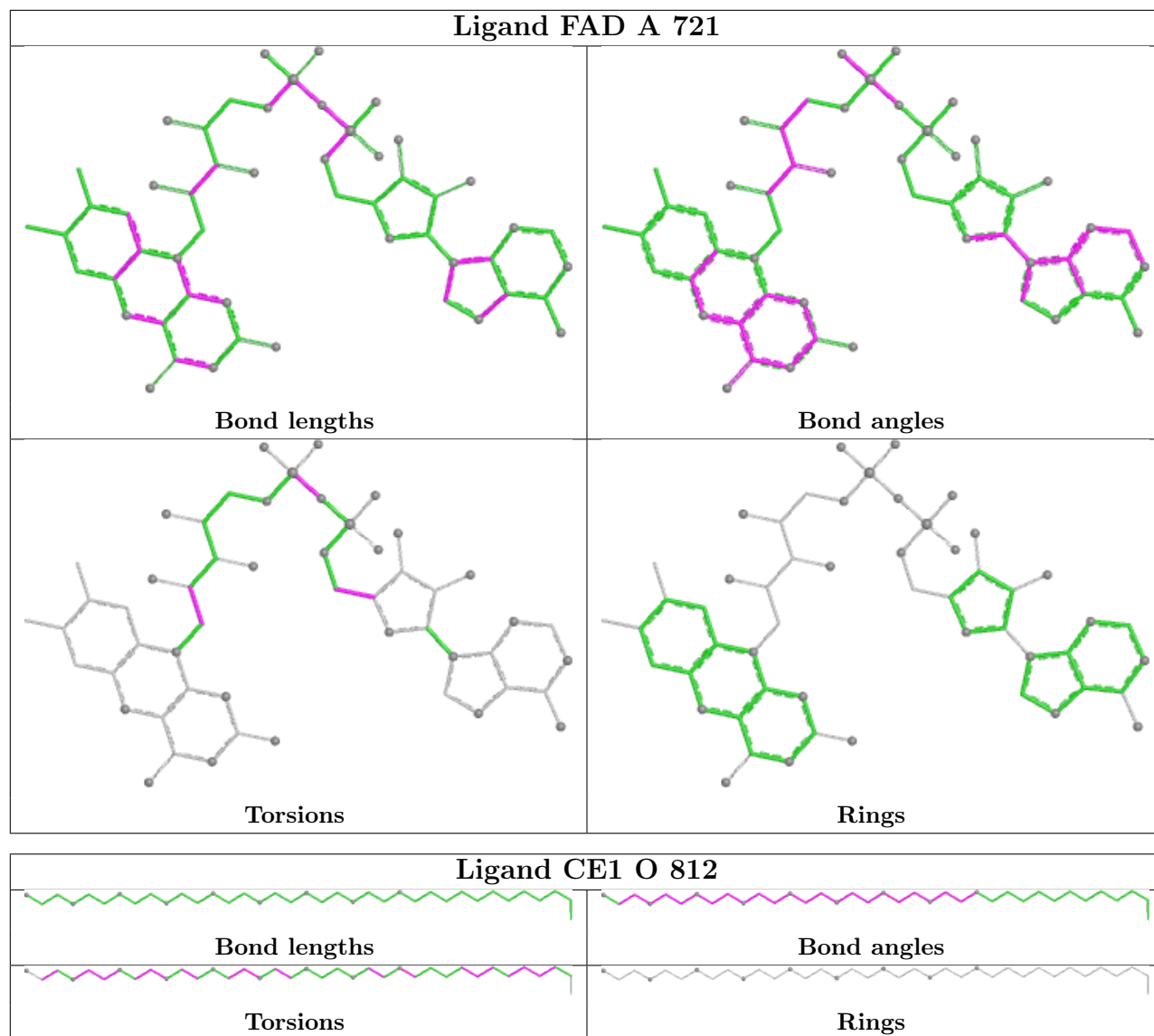
11 monomers are involved in 39 short contacts:

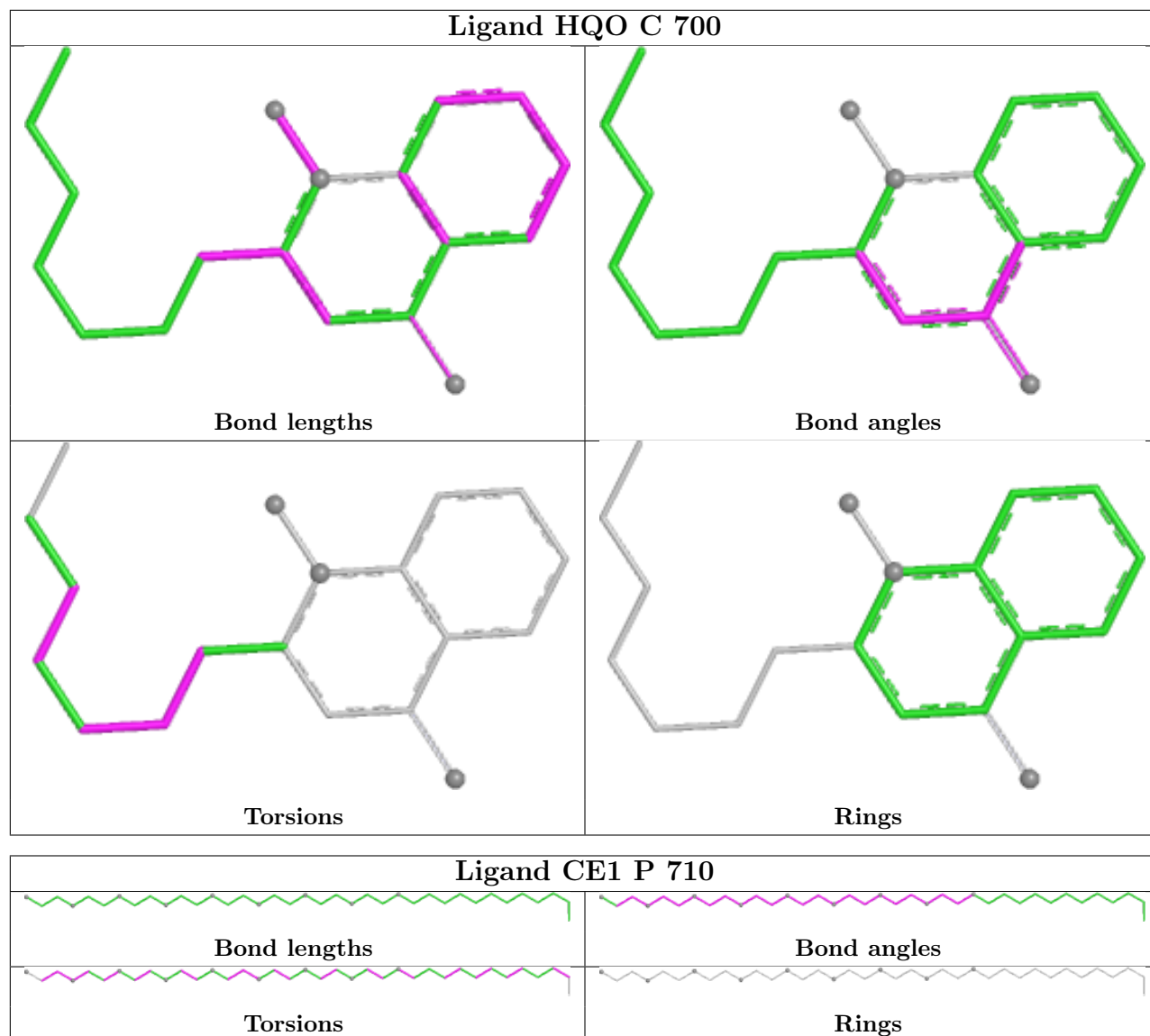
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	821	FAD	8	0
7	N	803	ACT	2	0
12	N	246	SF4	4	0
6	A	702	OAA	2	0
8	A	721	FAD	7	0
9	A	705	1PE	5	0
11	N	245	F3S	1	0
13	C	700	HQO	3	0
14	P	710	CE1	2	0
13	N	800	HQO	2	0
14	P	810	CE1	3	0

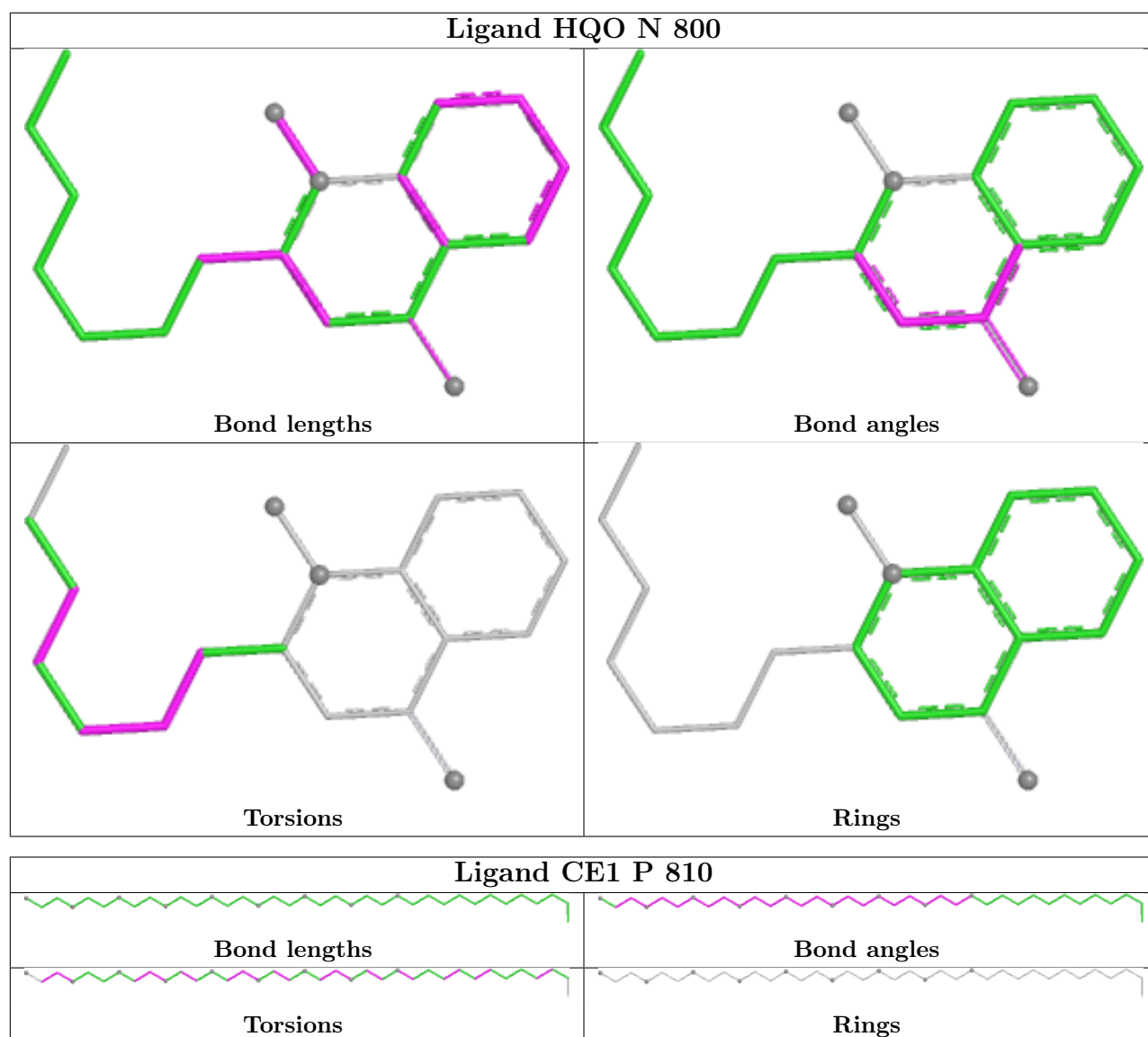
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand FAD M 821			
			
Bond lengths	Bond angles		
			
Torsions	Rings		
Ligand CE1 O 811			
			
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

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.