



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 04:32 am BST

PDB ID : 1KF6
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 following versions of software and data (see [references ⓘ](#)) 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) : 2.11

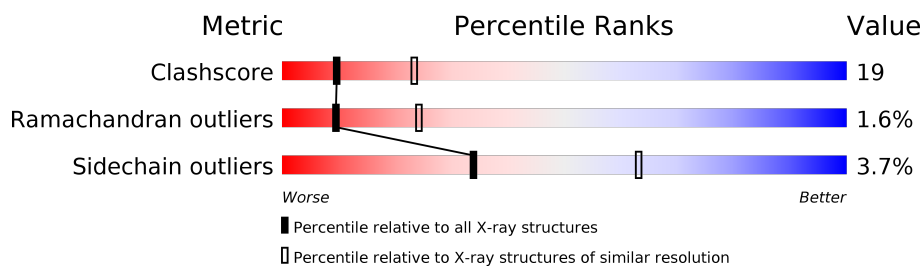
1 Overall quality at a glance

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 on 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	71% 22% . .
1	M	602	50% 42% . .
2	B	243	78% 20% .
2	N	243	51% 44% .
3	C	130	65% 29% . .
3	O	130	61% 35% 5%
4	D	119	61% 34% . .
4	P	119	49% 48% .

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	-
9	1PE	A	705	-	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			

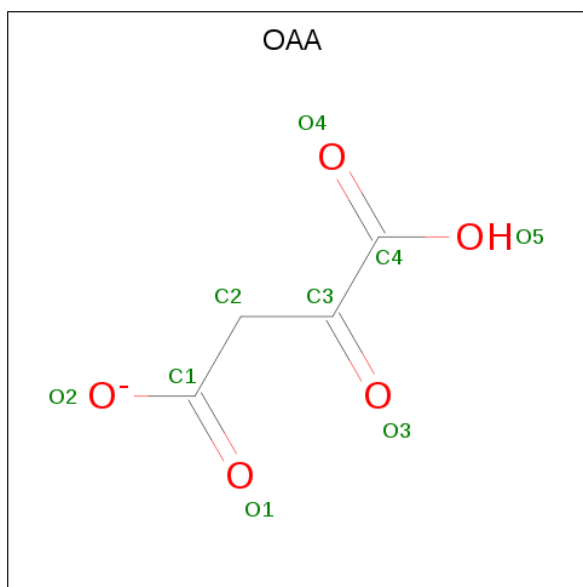
- Molecule 4 is a protein called FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN.

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 (three-letter code: K) (formula: K).

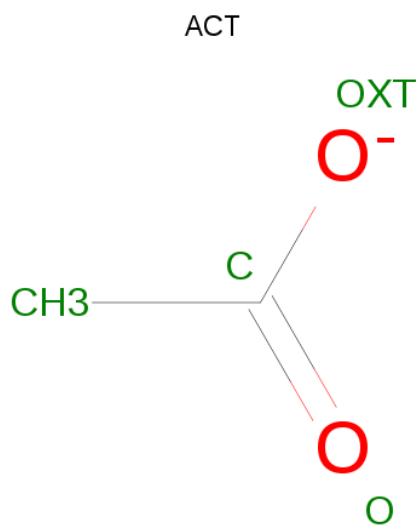
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	M	1	Total	K	0	0
			1	1		

- Molecule 6 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



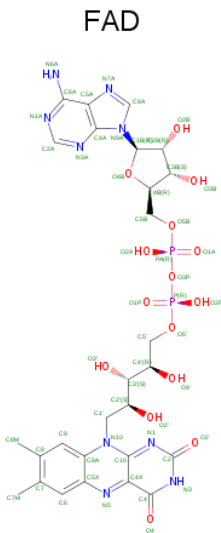
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	4	5		
6	M	1	Total	C	O	0	0
			9	4	5		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



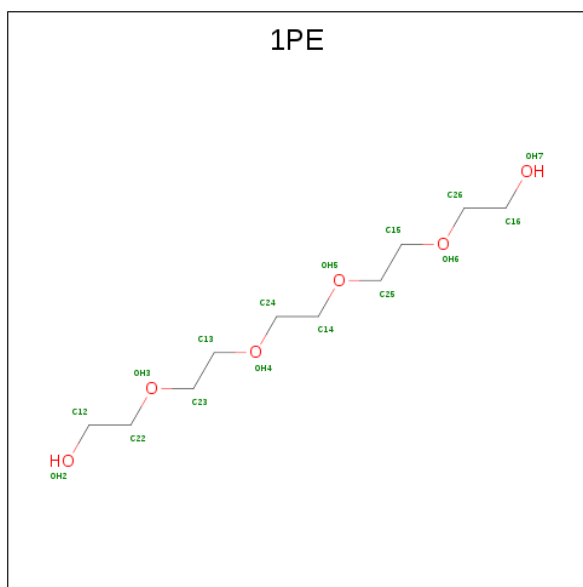
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	N	1	Total 4	C 2	O 2	0	0

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



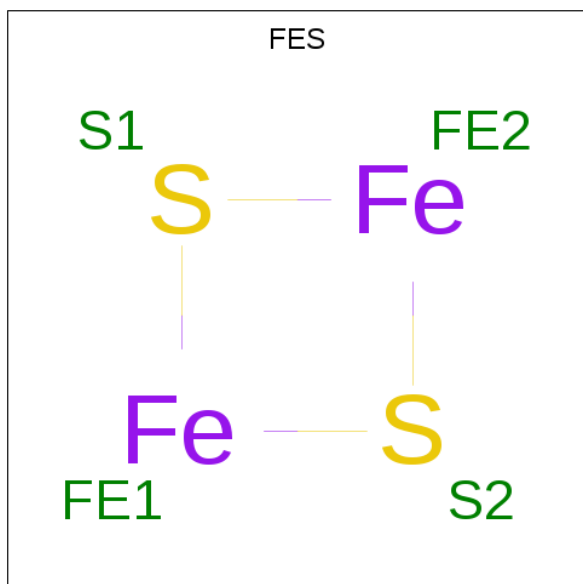
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
8	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



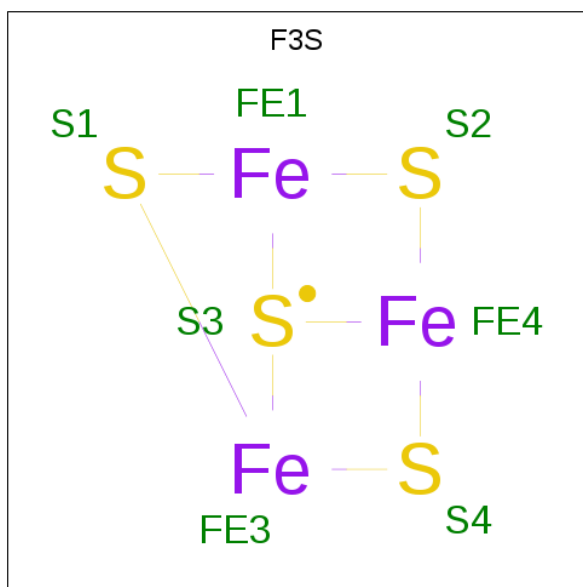
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			16	10	6		

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



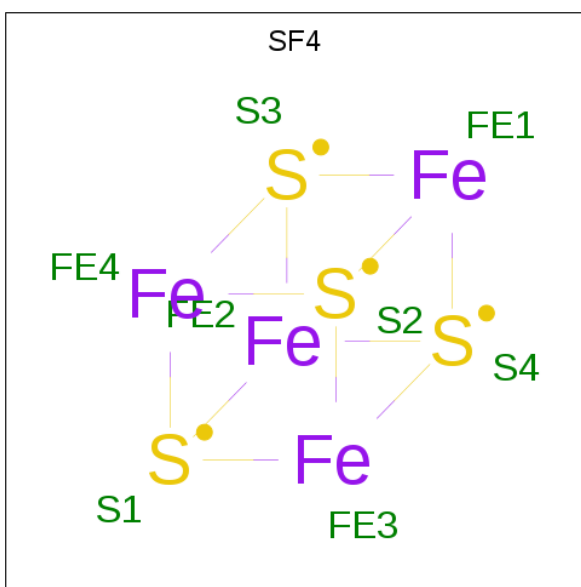
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			4	2	2		
10	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 11 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



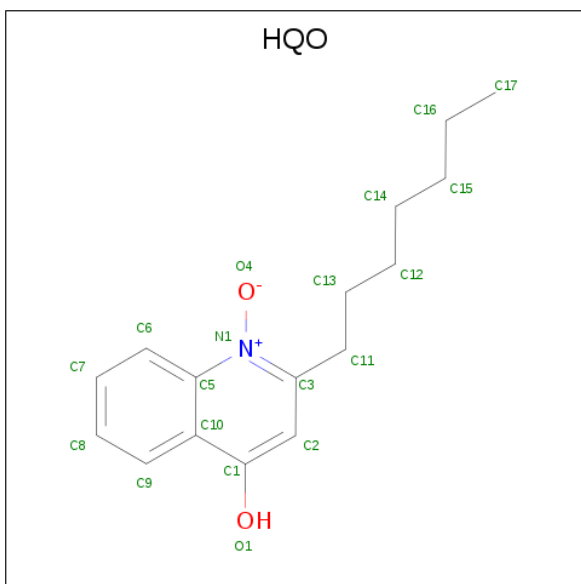
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			7	3	4		
11	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 12 is IRON/SULFUR CLUSTER (three-letter code: 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 (three-letter code: HQO) (formula: C₁₆H₂₁NO₂).



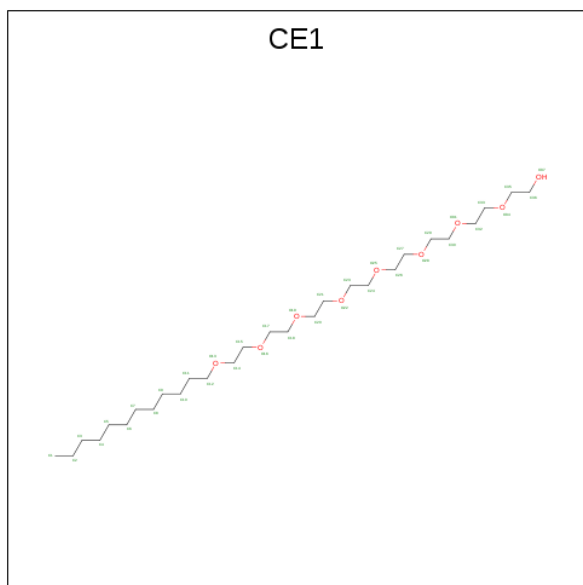
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			19	16	1	2		

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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 (three-letter code: 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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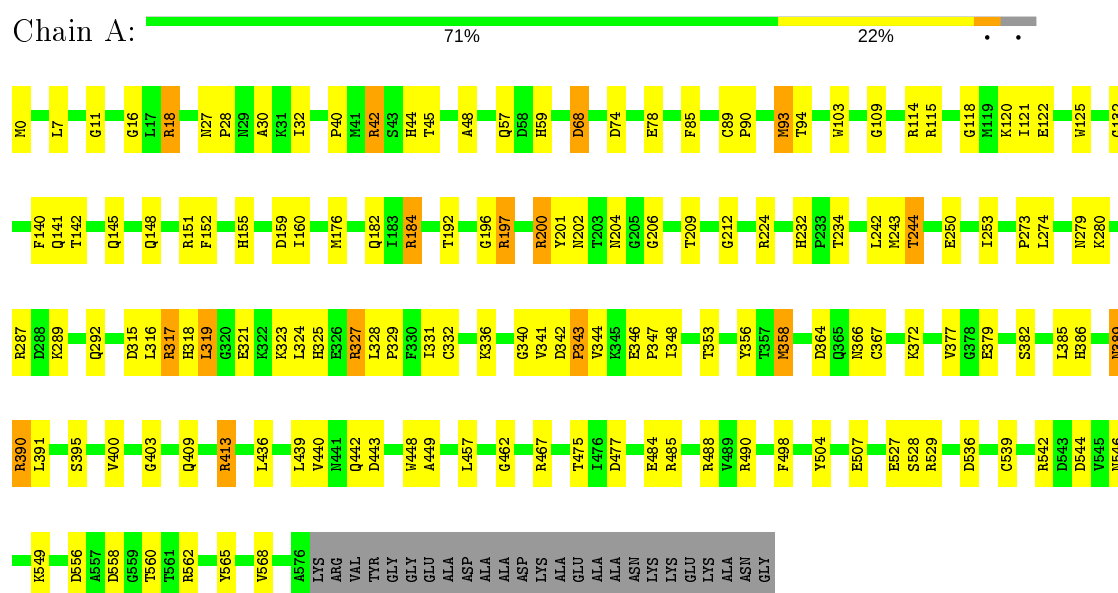
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	N	1	Total	O	0	0
			1	1		

3 Residue-property plots

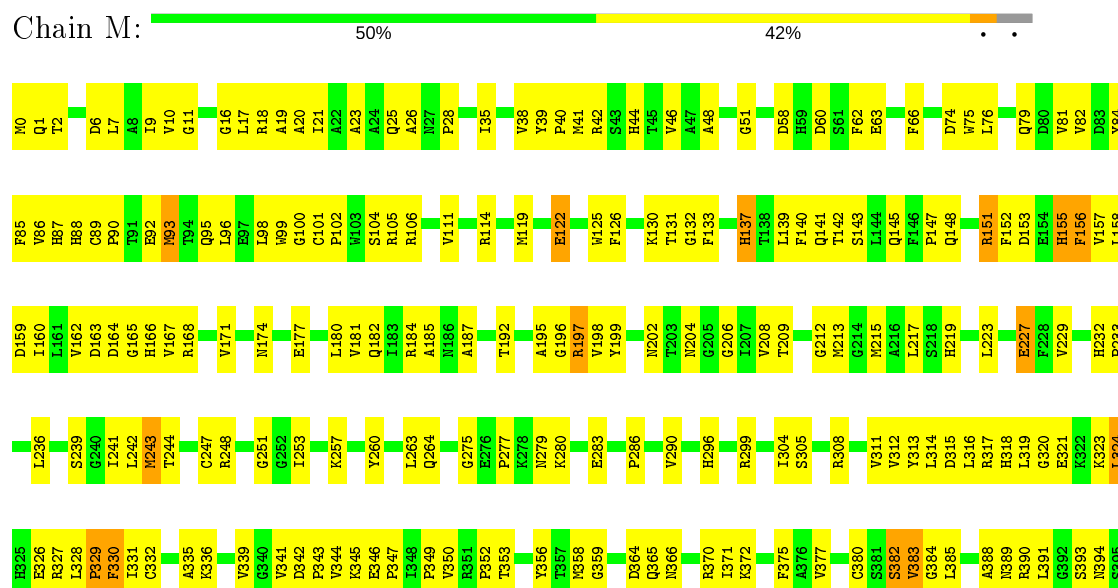
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

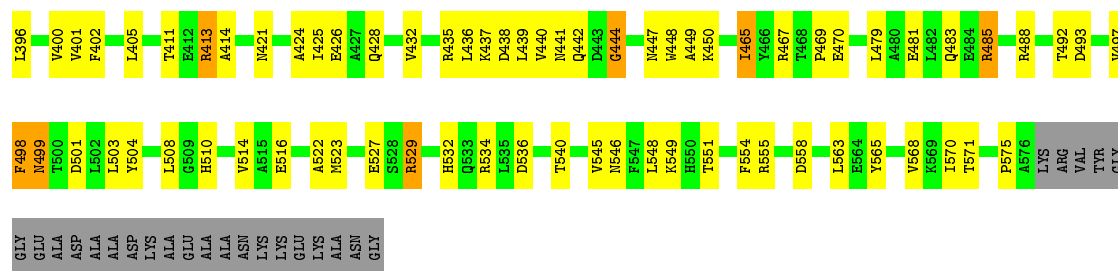
Note EDS was not executed.

• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN



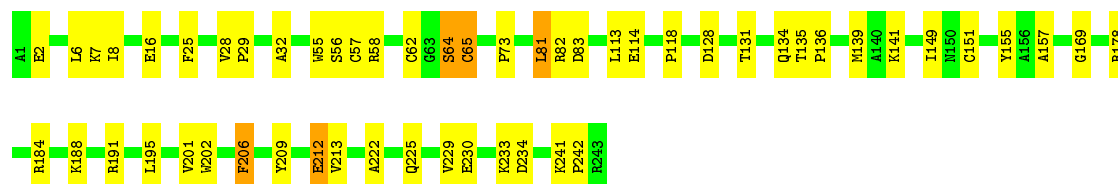
• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN





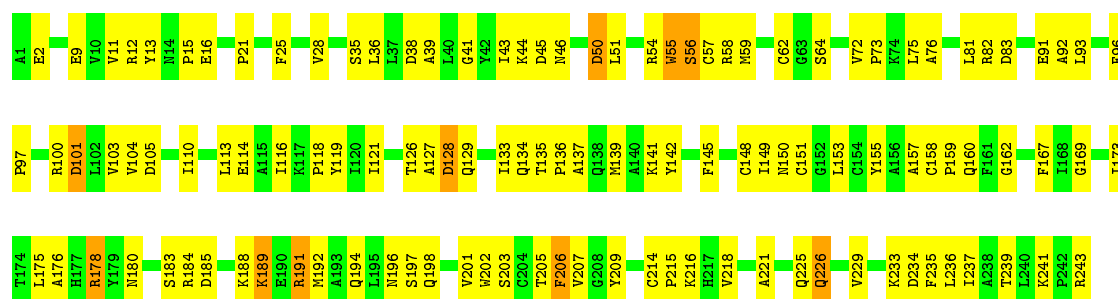
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain B: 78% 20% .



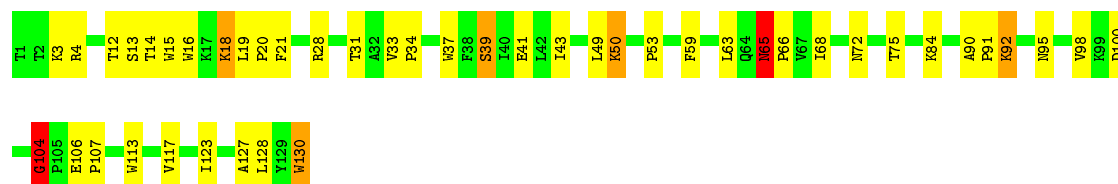
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain N: 51% 44% .



• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

Chain C: 65% 29% . .



• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

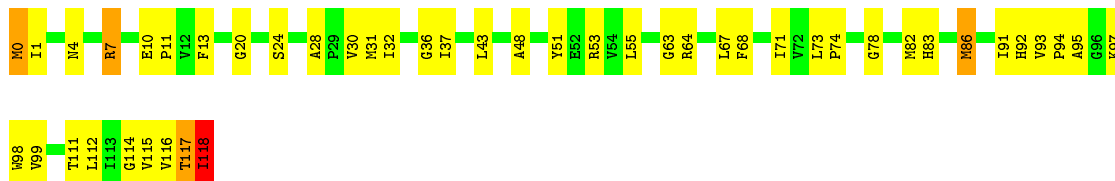
Chain O: 61% 35% 5%





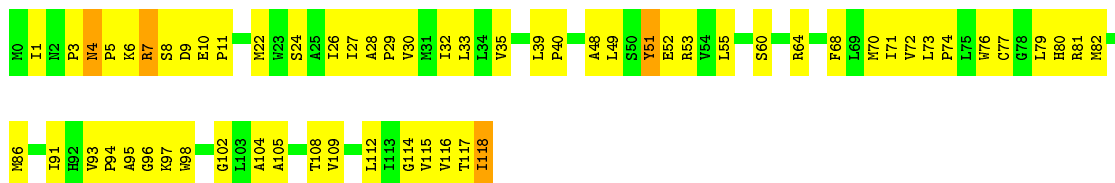
• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain D: 61% 34% . .



• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain P: 49% 48% .



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	96.50 Å 137.84 Å 273.45 Å 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: OAA, SF4, ACT, 1PE, F3S, FES, CE1, HQO, K, 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	0.81	0/4540	0.98	10/6139 (0.2%)
1	M	0.53	1/4540 (0.0%)	0.81	2/6139 (0.0%)
2	B	0.78	1/1931 (0.1%)	0.92	7/2617 (0.3%)
2	N	0.59	0/1931	0.81	1/2617 (0.0%)
3	C	0.77	3/1094 (0.3%)	0.87	2/1496 (0.1%)
3	O	0.68	3/1094 (0.3%)	0.79	1/1496 (0.1%)
4	D	0.78	1/956 (0.1%)	0.89	1/1303 (0.1%)
4	P	0.70	2/956 (0.2%)	0.82	0/1303
All	All	0.70	11/17042 (0.1%)	0.88	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
3	C	0	2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	118	ILE	C-OXT	11.65	1.45	1.23
4	P	118	ILE	C-OXT	8.01	1.38	1.23
2	B	65	CYS	CB-SG	-7.99	1.68	1.82
3	C	65	ASN	C-O	-7.42	1.09	1.23
3	O	104	GLY	C-O	-6.55	1.13	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ARG	NE-CZ-NH2	-7.24	116.68	120.30
4	D	7	ARG	NE-CZ-NH2	-7.24	116.68	120.30
2	B	191	ARG	NE-CZ-NH1	-6.88	116.86	120.30
3	C	28	ARG	NE-CZ-NH2	-6.71	116.95	120.30
2	B	65	CYS	N-CA-CB	-6.56	98.79	110.60

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	119	0
1	M	4448	0	4335	253	0
2	B	1888	0	1837	44	0
2	N	1888	0	1837	108	0
3	C	1058	0	1108	47	0
3	O	1058	0	1108	48	0
4	D	926	0	971	47	0
4	P	926	0	971	65	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	8	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	659	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 19.

The worst 5 of 659 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:HM82	1.21	1.44
1:M:44:HIS:NE2	8:M:821:FAD:HM82	1.18	1.42
1:A:44:HIS:NE2	8:A:721:FAD:C8M	1.89	1.33
1:M:44:HIS:NE2	8:M:821:FAD:C8M	1.98	1.27
1:A:44:HIS:CE1	8:A:721:FAD:HM82	1.86	1.08

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%)	22 46
1	M	575/602 (96%)	487 (85%)	75 (13%)	13 (2%)	6 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	241/243 (99%)	224 (93%)	16 (7%)	1 (0%)	34	60
2	N	241/243 (99%)	215 (89%)	20 (8%)	6 (2%)	5	14
3	C	128/130 (98%)	120 (94%)	4 (3%)	4 (3%)	4	9
3	O	128/130 (98%)	114 (89%)	12 (9%)	2 (2%)	9	24
4	D	117/119 (98%)	111 (95%)	3 (3%)	3 (3%)	5	13
4	P	117/119 (98%)	102 (87%)	14 (12%)	1 (1%)	17	40
All	All	2122/2188 (97%)	1914 (90%)	174 (8%)	34 (2%)	9	24

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%)	446 (97%)	14 (3%)	41	70
1	M	460/475 (97%)	437 (95%)	23 (5%)	24	51
2	B	205/205 (100%)	199 (97%)	6 (3%)	42	71
2	N	205/205 (100%)	195 (95%)	10 (5%)	25	52
3	C	111/111 (100%)	107 (96%)	4 (4%)	35	64
3	O	111/111 (100%)	108 (97%)	3 (3%)	44	74
4	D	97/97 (100%)	94 (97%)	3 (3%)	40	69
4	P	97/97 (100%)	95 (98%)	2 (2%)	53	80
All	All	1746/1776 (98%)	1681 (96%)	65 (4%)	34	63

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	122	GLU
1	M	164	ASP
3	O	5	LYS
1	M	126	PHE
1	M	155	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	174	ASN
1	M	409	GLN
2	N	186	HIS
1	M	292	GLN
1	M	421	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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
11	F3S	N	245	2	0,9,9	0.00	-	-		
10	FES	N	244	2	0,4,4	0.00	-	-		
11	F3S	B	245	2	0,9,9	0.00	-	-		
7	ACT	N	803	-	1,3,3	3.02	1 (100%)	0,3,3	0.00	-
13	HQO	N	800	-	20,20,20	3.05	8 (40%)	18,26,26	1.18	1 (5%)
14	CE1	O	813	-	36,36,36	1.18	0	35,35,35	1.95	15 (42%)
12	SF4	N	246	2	0,12,12	0.00	-	-		
14	CE1	P	710	-	36,36,36	1.10	0	35,35,35	1.91	15 (42%)
14	CE1	P	810	-	36,36,36	1.10	0	35,35,35	1.99	15 (42%)
12	SF4	B	246	2	0,12,12	0.00	-	-		
8	FAD	A	721	-	51,58,58	1.77	8 (15%)	60,89,89	1.69	11 (18%)
6	OAA	A	702	-	2,8,8	2.22	1 (50%)	2,10,10	2.32	1 (50%)
6	OAA	M	802	-	2,8,8	2.20	1 (50%)	2,10,10	2.32	1 (50%)
7	ACT	A	703	-	1,3,3	1.95	0	0,3,3	0.00	-
14	CE1	O	811	-	36,36,36	1.11	0	35,35,35	1.97	15 (42%)
9	1PE	A	705	-	15,15,15	1.63	0	14,14,14	2.29	10 (71%)
8	FAD	M	821	-	51,58,58	1.67	9 (17%)	60,89,89	1.62	7 (11%)
10	FES	B	244	2	0,4,4	0.00	-	-		
13	HQO	C	700	-	20,20,20	3.05	8 (40%)	18,26,26	1.18	1 (5%)
14	CE1	O	812	-	36,36,36	1.11	0	35,35,35	1.89	15 (42%)
7	ACT	B	704	-	1,3,3	3.25	1 (100%)	0,3,3	0.00	-

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
11	F3S	N	245	2	-	-	0/3/3/3
10	FES	N	244	2	-	-	0/1/1/1
14	CE1	O	813	-	-	14/34/34/34	-
6	OAA	M	802	-	-	2/2/8/8	-
12	SF4	N	246	2	-	-	0/6/5/5
14	CE1	P	710	-	-	17/34/34/34	-
14	CE1	P	810	-	-	16/34/34/34	-
12	SF4	B	246	2	-	-	0/6/5/5
8	FAD	A	721	-	-	6/30/50/50	0/6/6/6
6	OAA	A	702	-	-	2/2/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	F3S	B	245	2	-	-	0/3/3/3
14	CE1	O	811	-	-	18/34/34/34	-
9	1PE	A	705	-	-	8/13/13/13	-
8	FAD	M	821	-	-	5/30/50/50	0/6/6/6
10	FES	B	244	2	-	-	0/1/1/1
13	HQO	C	700	-	-	3/7/7/7	0/2/2/2
14	CE1	O	812	-	-	18/34/34/34	-
13	HQO	N	800	-	-	3/7/7/7	0/2/2/2

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	800	HQO	O4-N1	-11.24	1.23	1.38
13	C	700	HQO	O4-N1	-11.24	1.23	1.38
8	A	721	FAD	C4-N3	6.05	1.43	1.33
8	M	821	FAD	C4-N3	5.43	1.42	1.33
8	A	721	FAD	C10-N1	4.59	1.39	1.33

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	721	FAD	C4X-N5-C5X	6.33	123.09	116.77
8	M	821	FAD	C4X-N5-C5X	6.25	123.02	116.77
8	M	821	FAD	N3A-C2A-N1A	-5.72	119.73	128.68
8	A	721	FAD	C4-N3-C2	4.72	119.13	115.14
14	P	810	CE1	O28-C27-C26	4.64	131.30	110.39

There are no chirality outliers.

5 of 112 torsion outliers are listed below:

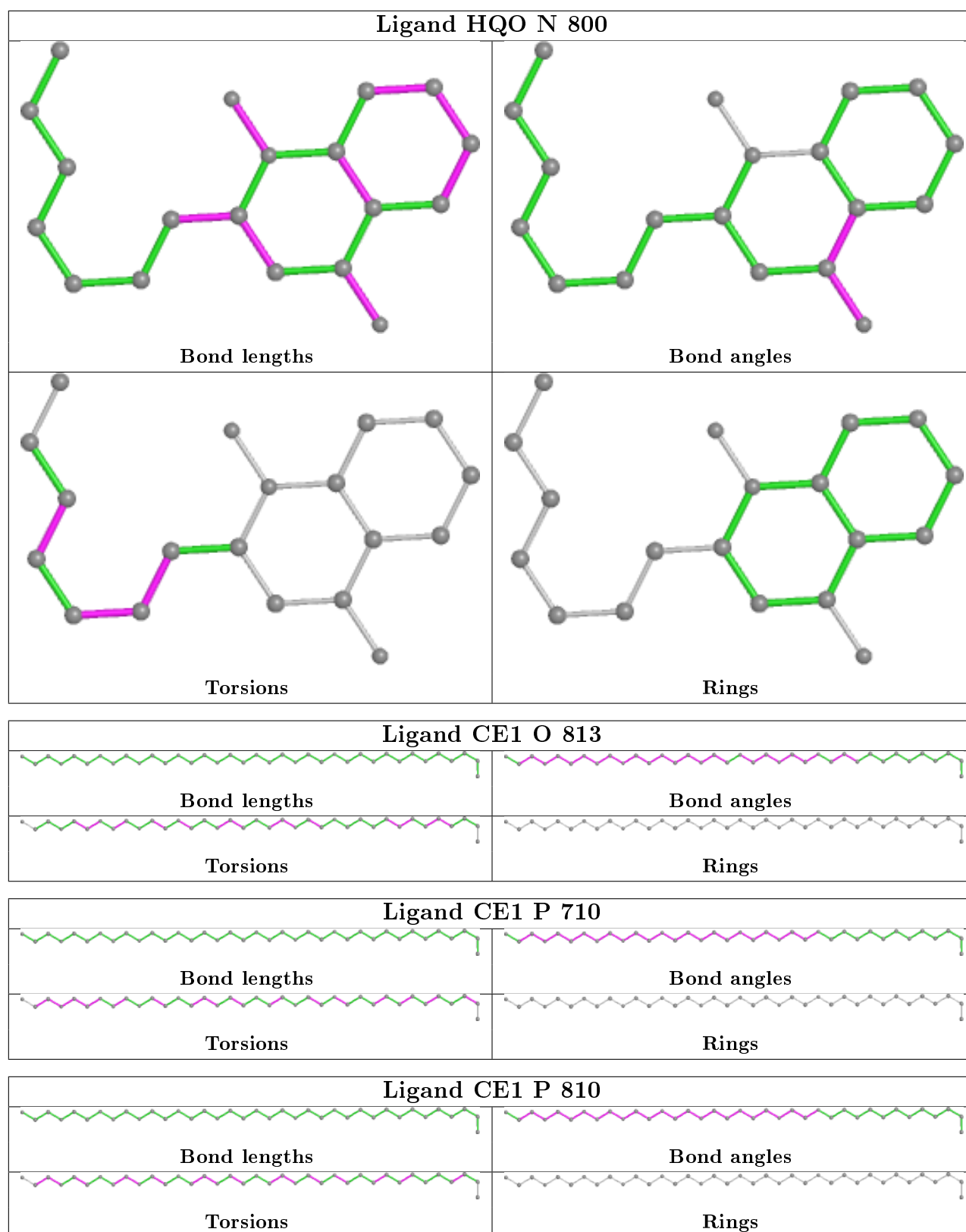
Mol	Chain	Res	Type	Atoms
8	A	721	FAD	N10-C1'-C2'-O2'
8	A	721	FAD	N10-C1'-C2'-C3'
8	A	721	FAD	PA-O3P-P-O5'
8	M	821	FAD	N10-C1'-C2'-O2'
8	M	821	FAD	N10-C1'-C2'-C3'

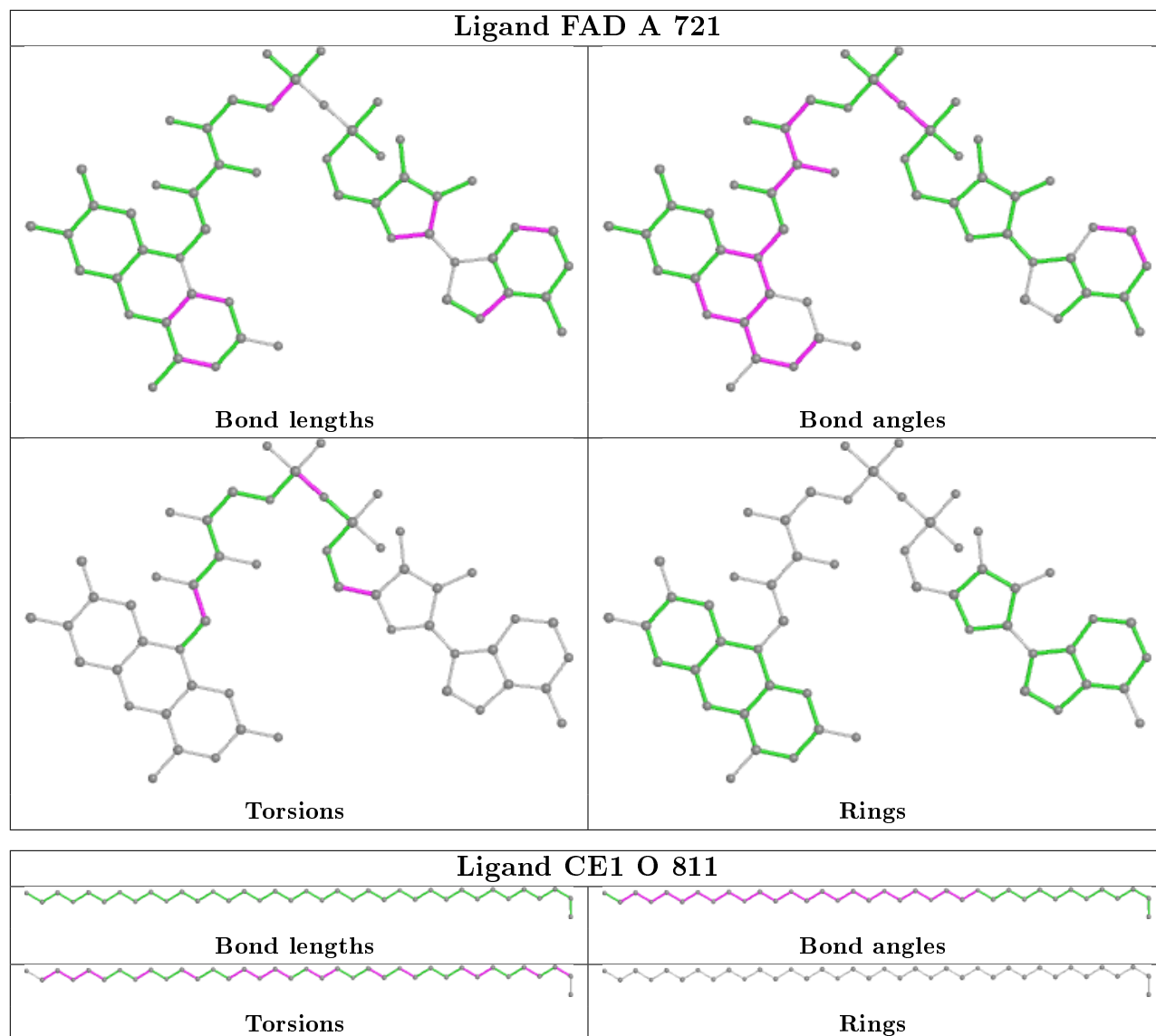
There are no ring outliers.

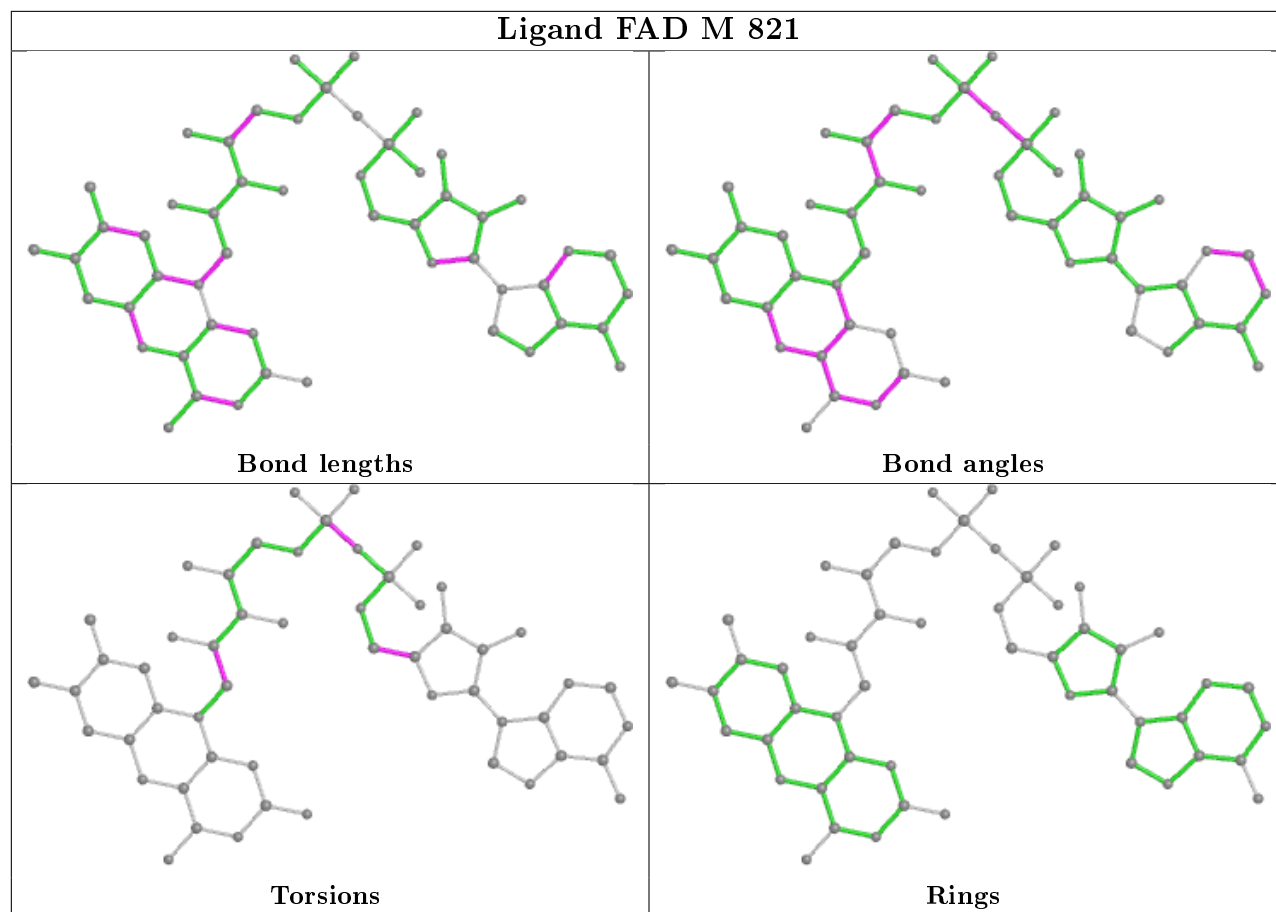
11 monomers are involved in 40 short contacts:

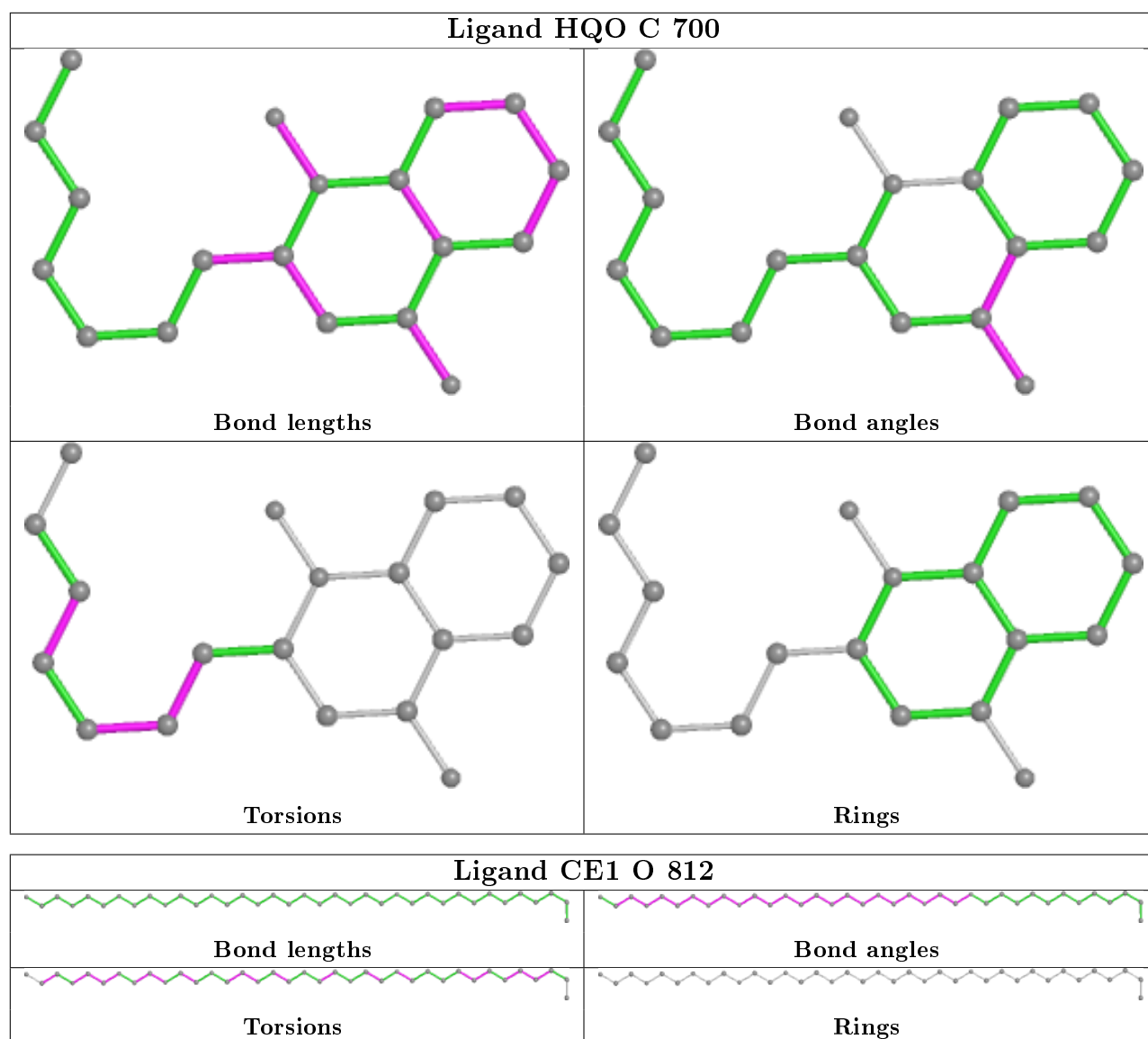
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	N	245	F3S	1	0
7	N	803	ACT	2	0
13	N	800	HQO	2	0
12	N	246	SF4	4	0
14	P	710	CE1	2	0
14	P	810	CE1	3	0
8	A	721	FAD	8	0
6	A	702	OAA	2	0
9	A	705	1PE	5	0
8	M	821	FAD	8	0
13	C	700	HQO	3	0

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.









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.