



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 22, 2019 – 07:40 PM EDT

PDB ID : 3ZFS
EMDB ID: : EMD-2097
Title : Cryo-EM structure of the F420-reducing NiFe-hydrogenase from a
methanogenic archaeon with bound substrate
Authors : Mills, D.J.; Vitt, S.; Strauss, M.; Shima, S.; Vonck, J.
Deposited on : 2012-12-12
Resolution : 4.00 Å(reported)
Based on PDB ID : 2WPN

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

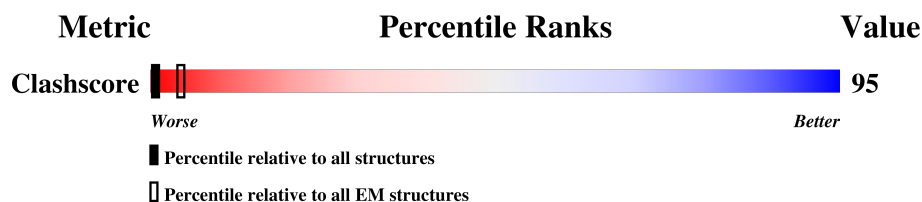
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 4.00 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)	EM structures (#Entries)
Clashscore	136327	1886

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	405	 86% 9% 5%
2	B	275	 64% 14% 22%
3	C	281	 78% 21% .

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
7	SF4	B	300	-	-	X	-
7	SF4	C	303	-	-	X	-
8	F42	C	285	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 985 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 F420-REDUCING HYDROGENASE, SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	385	Total	C	0	385
			385	385		

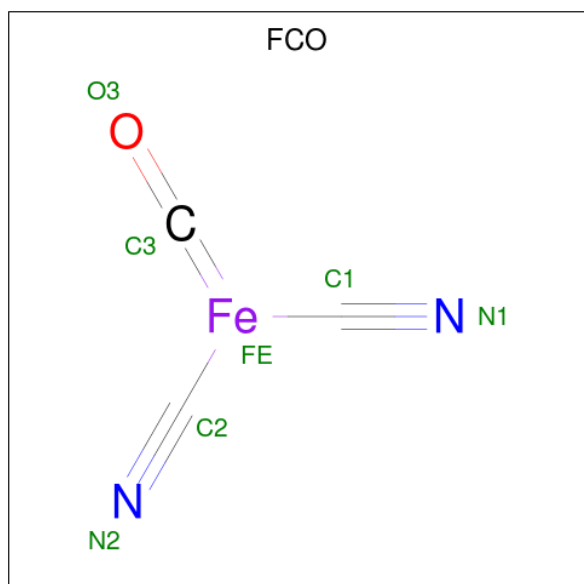
- Molecule 2 is a protein called F420-REDUCING HYDROGENASE, SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	B	215	Total	C	0	215
			215	215		

- Molecule 3 is a protein called F420-REDUCING HYDROGENASE, SUBUNIT BETA.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	C	278	Total	C	0	278
			278	278		

- Molecule 4 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Fe	0
			1	1	

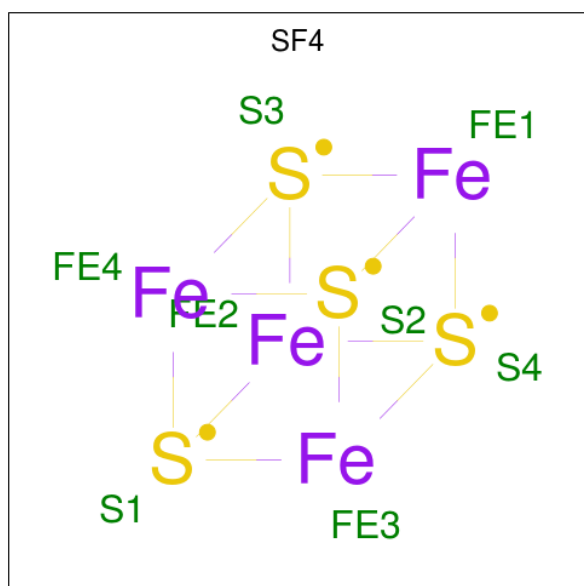
- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ni	0
			1	1	

- Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe).

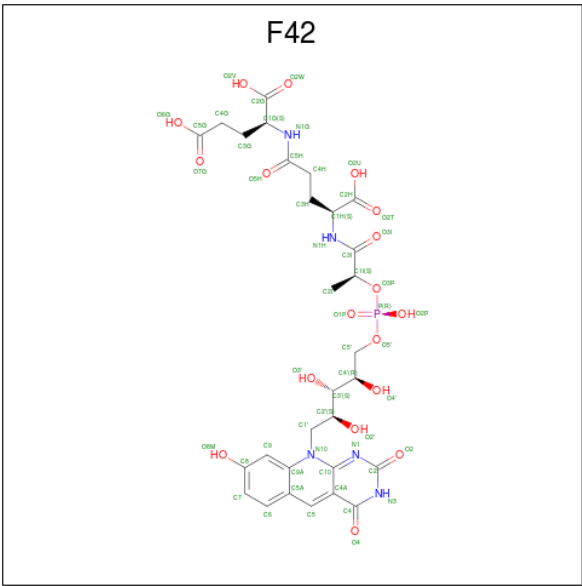
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Fe	0
			1	1	

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



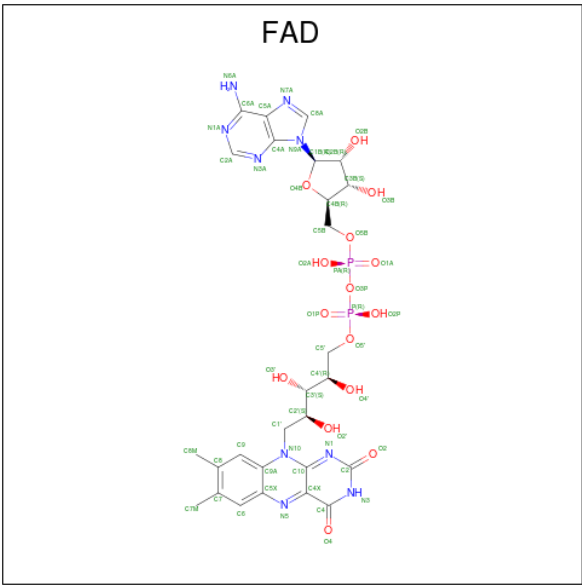
Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	Fe	S	0
			24	12	12	
7	B	1	Total	Fe	S	0
			24	12	12	
7	B	1	Total	Fe	S	0
			24	12	12	
7	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 8 is COENZYME F420 (three-letter code: F42) (formula: C₂₉H₃₆N₅O₁₈P).



Mol	Chain	Residues	Atoms				AltConf
8	C	1	Total	C	N	O	0
			19	13	3	3	

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	97290	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PER MICROGRAPH	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1650	Depositor
Maximum defocus (nm)	3820	Depositor
Magnification	61400	Depositor
Image detector	KODAK SO-163 FILM	Depositor

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: NI, F42, SF4, FE2, FAD, FCO

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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 [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	385	0	0	21	0
2	B	215	0	0	23	0
3	C	278	0	0	49	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	B	24	0	0	3	0
7	C	8	0	0	3	0
8	C	19	0	8	8	0
9	C	53	0	30	12	0
All	All	985	0	38	97	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 95.

All (97) 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)
3:C:25:ASP:CA	9:C:304:FAD:C5'	1.78	1.58
3:C:104:CYS:CA	7:C:303:SF4:S3	2.04	1.45
3:C:25:ASP:CA	9:C:304:FAD:O4'	1.71	1.38
3:C:25:ASP:CA	9:C:304:FAD:C4'	2.11	1.28
3:C:26:GLY:CA	9:C:304:FAD:H51A	1.85	1.06
9:C:304:FAD:H9	9:C:304:FAD:O2'	1.55	1.04
2:B:132:CYS:CA	2:B:136:GLY:CA	2.38	1.01
3:C:209:SER:CA	8:C:285:F42:H5	1.93	0.98
9:C:304:FAD:C2'	9:C:304:FAD:H9	1.95	0.96
3:C:209:SER:CA	8:C:285:F42:C5	2.47	0.93
3:C:26:GLY:CA	9:C:304:FAD:C5B	2.47	0.91
3:C:211:GLY:CA	3:C:249:PRO:CA	2.57	0.83
3:C:102:ILE:CA	3:C:105:GLN:CA	2.60	0.79
1:A:199:PRO:CA	1:A:200:GLU:CA	2.62	0.78
3:C:72:ALA:CA	9:C:304:FAD:H3B	2.14	0.77
3:C:210:VAL:CA	8:C:285:F42:C5	2.64	0.74
9:C:304:FAD:C2'	9:C:304:FAD:C9	2.60	0.74
3:C:215:GLY:CA	3:C:216:TRP:CA	2.70	0.70
1:A:369:TYR:CA	1:A:370:GLY:CA	2.71	0.69
2:B:159:ALA:CA	2:B:160:ASP:CA	2.71	0.68
9:C:304:FAD:H2'	9:C:304:FAD:C9	2.24	0.66
2:B:109:ASP:CA	2:B:110:GLU:CA	2.74	0.66
3:C:210:VAL:CA	8:C:285:F42:H5	2.24	0.66
2:B:59:GLY:CA	7:B:300:SF4:S2	2.84	0.66
1:A:223:ASP:CA	1:A:224:LEU:CA	2.75	0.65
3:C:151:LEU:CA	3:C:152:GLY:CA	2.75	0.64
3:C:43:GLU:CA	3:C:44:GLY:CA	2.74	0.64
2:B:163:ASP:CA	2:B:164:VAL:CA	2.76	0.64
3:C:23:ALA:CA	3:C:24:GLN:CA	2.76	0.63
3:C:40:GLY:CA	3:C:41:ILE:CA	2.77	0.63
3:C:209:SER:CA	8:C:285:F42:C5A	2.77	0.63
3:C:190:ALA:CA	3:C:191:GLY:CA	2.77	0.62
2:B:47:PRO:CA	2:B:48:ARG:CA	2.78	0.62
1:A:8:SER:CA	1:A:9:PRO:CA	2.78	0.62
3:C:42:ILE:CA	3:C:43:GLU:CA	2.77	0.62
3:C:48:ALA:CA	3:C:49:GLY:CA	2.77	0.62
1:A:363:GLU:CA	1:A:364:GLY:CA	2.77	0.62
2:B:97:ASP:CA	2:B:124:LYS:CA	2.78	0.62
3:C:134:CYS:CA	3:C:135:MET:CA	2.78	0.61
2:B:164:VAL:CA	2:B:165:ASP:CA	2.78	0.61
3:C:249:PRO:CA	3:C:250:GLY:CA	2.78	0.61
2:B:201:GLY:CA	2:B:202:TYR:CA	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:214:ASP:CA	3:C:215:GLY:CA	2.78	0.61
1:A:368:GLU:CA	1:A:369:TYR:CA	2.78	0.61
2:B:135:THR:CA	2:B:136:GLY:CA	2.78	0.61
2:B:147:GLN:CA	2:B:148:ALA:CA	2.78	0.61
3:C:209:SER:CA	8:C:285:F42:C6	2.78	0.61
1:A:36:SER:CA	1:A:37:ILE:CA	2.79	0.60
2:B:205:ALA:CA	2:B:206:CYS:CA	2.80	0.60
2:B:56:GLY:CA	7:B:300:SF4:S3	2.90	0.60
2:B:136:GLY:CA	2:B:137:CYS:CA	2.80	0.59
1:A:235:TRP:CA	1:A:236:TYR:CA	2.80	0.59
2:B:69:ASP:CA	2:B:70:ILE:CA	2.80	0.59
1:A:202:LEU:CA	1:A:203:GLY:CA	2.81	0.59
3:C:123:ALA:CA	3:C:124:ASP:CA	2.81	0.59
2:B:212:THR:CA	2:B:213:LYS:CA	2.80	0.59
3:C:116:PRO:CA	3:C:117:PHE:CA	2.80	0.59
1:A:215:ILE:CA	1:A:216:TYR:CA	2.81	0.59
3:C:101:ALA:CA	3:C:102:ILE:CA	2.81	0.59
1:A:362:THR:CA	1:A:363:GLU:CA	2.81	0.58
1:A:224:LEU:CA	1:A:225:ASP:CA	2.82	0.58
2:B:66:GLU:CA	2:B:67:ASN:CA	2.82	0.58
3:C:15:THR:CA	3:C:16:ASP:CA	2.83	0.57
3:C:204:ASP:CA	3:C:205:VAL:CA	2.82	0.56
3:C:236:ALA:CA	3:C:237:GLY:CA	2.83	0.56
1:A:148:GLY:CA	1:A:149:ILE:CA	2.83	0.56
2:B:68:TYR:CA	2:B:69:ASP:CA	2.84	0.56
3:C:93:GLY:CA	3:C:94:ILE:CA	2.83	0.56
3:C:247:VAL:CA	3:C:248:LYS:CA	2.84	0.56
3:C:169:TRP:CA	3:C:170:VAL:CA	2.83	0.56
3:C:199:VAL:CA	3:C:200:ALA:CA	2.84	0.55
3:C:209:SER:CA	9:C:304:FAD:O2	2.54	0.55
2:B:210:LEU:CA	2:B:211:GLN:CA	2.84	0.55
1:A:207:GLN:CA	1:A:208:PRO:CA	2.84	0.55
1:A:203:GLY:CA	1:A:204:VAL:CA	2.84	0.55
3:C:158:VAL:CA	3:C:159:GLU:CA	2.85	0.55
3:C:186:GLY:CA	3:C:187:TYR:CA	2.86	0.54
3:C:277:LEU:CA	3:C:278:PRO:CA	2.85	0.54
2:B:250:ILE:CA	2:B:251:LYS:CA	2.85	0.53
1:A:231:MET:CA	1:A:232:PRO:CA	2.86	0.53
2:B:224:GLY:CA	7:B:302:SF4:S1	2.97	0.53
1:A:217:GLY:CA	1:A:218:ASP:CA	2.87	0.52
3:C:92:TYR:CA	3:C:93:GLY:CA	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:CA	1:A:220:THR:CA	2.87	0.52
3:C:134:CYS:CA	7:C:303:SF4:S4	2.98	0.52
2:B:165:ASP:CA	2:B:166:LEU:CA	2.89	0.50
3:C:153:VAL:CA	3:C:154:SER:CA	2.91	0.49
3:C:134:CYS:CA	7:C:303:SF4:S1	3.01	0.48
3:C:210:VAL:CA	8:C:285:F42:H6	2.43	0.48
1:A:38:THR:CA	1:A:39:PRO:CA	2.92	0.48
3:C:150:LYS:CA	3:C:151:LEU:CA	2.93	0.47
3:C:161:MET:CA	3:C:170:VAL:CA	2.94	0.46
2:B:171:CYS:CA	2:B:172:PRO:CA	2.94	0.45
1:A:314:ARG:CA	1:A:315:GLY:CA	2.95	0.44
3:C:25:ASP:CA	9:C:304:FAD:O3P	2.67	0.42
3:C:210:VAL:CA	8:C:285:F42:C6	2.99	0.41
1:A:267:GLU:CA	1:A:268:PHE:CA	2.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is modelled with single atom and 2 are monoatomic - leaving 6 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	$\# Z > 2$
7	SF4	B	300	-	0,12,12	0.00	-	-		
7	SF4	B	301	-	0,12,12	0.00	-	-		
7	SF4	B	302	-	0,12,12	0.00	-	-		
8	F42	C	285	-	19,21,55	5.19	12 (63%)	18,31,79	4.54	13 (72%)
7	SF4	C	303	-	0,12,12	0.00	-	-		
9	FAD	C	304	-	50,58,58	1.87	6 (12%)	58,89,89	1.92	12 (20%)

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
7	SF4	B	300	-	-	-	0/6/5/5
7	SF4	B	301	-	-	-	0/6/5/5
7	SF4	B	302	-	-	-	0/6/5/5
8	F42	C	285	-	-	2/2/2/53	0/3/3/3
7	SF4	C	303	-	-	-	0/6/5/5
9	FAD	C	304	-	-	20/30/50/50	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	304	FAD	C4X-C10	9.53	1.48	1.38
8	C	285	F42	C10-N1	-9.20	1.35	1.46
8	C	285	F42	C5-C4A	-8.79	1.40	1.53
8	C	285	F42	C4A-C4	-7.90	1.40	1.51
8	C	285	F42	C5A-C9A	-6.77	1.40	1.53
8	C	285	F42	C9A-N10	-6.59	1.36	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	285	F42	C9-C9A	-6.19	1.40	1.53
8	C	285	F42	C9-C8	-6.07	1.40	1.51
8	C	285	F42	C5-C5A	-5.78	1.40	1.53
8	C	285	F42	C6-C5A	-5.39	1.40	1.53
8	C	285	F42	C7-C6	-5.36	1.39	1.52
8	C	285	F42	C7-C8	-4.67	1.40	1.51
9	C	304	FAD	C4-C4X	4.18	1.48	1.41
9	C	304	FAD	C9A-C5X	3.54	1.49	1.42
9	C	304	FAD	C8-C7	3.28	1.49	1.40
9	C	304	FAD	C5A-C4A	3.10	1.47	1.40
8	C	285	F42	O8M-C8	-2.09	1.37	1.43
9	C	304	FAD	C9A-N10	2.08	1.41	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	285	F42	C5-C4A-C10	8.87	118.78	107.74
9	C	304	FAD	C4-N3-C2	8.41	122.24	115.14
8	C	285	F42	C9-C8-C7	8.09	120.33	110.54
8	C	285	F42	C5-C5A-C9A	6.40	118.92	110.04
8	C	285	F42	C5-C4A-C4	5.53	122.36	111.13
8	C	285	F42	O8M-C8-C9	5.37	120.52	109.86
8	C	285	F42	C4-N3-C2	-4.86	119.74	126.25
8	C	285	F42	C6-C7-C8	4.80	119.80	111.57
9	C	304	FAD	C4-C4X-C10	-4.57	116.57	119.95
8	C	285	F42	C5-C5A-C6	4.07	120.13	112.68
8	C	285	F42	C6-C5A-C9A	4.07	120.95	109.72
9	C	304	FAD	C4X-N5-C5X	3.85	120.72	116.77
9	C	304	FAD	P-O3P-PA	-3.81	120.46	132.57
9	C	304	FAD	C4X-C4-N3	-3.58	118.49	123.47
8	C	285	F42	O8M-C8-C7	3.56	119.15	110.13
8	C	285	F42	C7-C6-C5A	3.30	119.78	112.23
9	C	304	FAD	C4-C4X-N5	3.22	122.14	118.59
9	C	304	FAD	N3A-C2A-N1A	-3.07	123.73	128.68
8	C	285	F42	N3-C2-N1	2.86	119.20	116.13
9	C	304	FAD	C1'-N10-C9A	2.83	120.77	118.31
9	C	304	FAD	C4A-C5A-N7A	-2.69	106.60	109.40
9	C	304	FAD	C9A-N10-C10	-2.59	118.39	121.77
9	C	304	FAD	C1'-N10-C10	2.42	120.83	118.46
8	C	285	F42	O2-C2-N1	-2.40	118.05	122.94
9	C	304	FAD	C5X-C9A-N10	2.34	119.50	117.71

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	285	F42	C2'-C1'-N10-C9A
9	C	304	FAD	C5B-O5B-PA-O3P
9	C	304	FAD	C3B-C4B-C5B-O5B
9	C	304	FAD	C2'-C1'-N10-C9A
9	C	304	FAD	C2'-C1'-N10-C10
9	C	304	FAD	N10-C1'-C2'-O2'
9	C	304	FAD	N10-C1'-C2'-C3'
9	C	304	FAD	C2'-C3'-C4'-O4'
9	C	304	FAD	O3'-C3'-C4'-O4'
9	C	304	FAD	O3'-C3'-C4'-C5'
9	C	304	FAD	C3'-C4'-C5'-O5'
9	C	304	FAD	O4'-C4'-C5'-O5'
9	C	304	FAD	C5'-O5'-P-O1P
9	C	304	FAD	C5'-O5'-P-O2P
9	C	304	FAD	C5'-O5'-P-O3P
9	C	304	FAD	O4B-C4B-C5B-O5B
9	C	304	FAD	C2'-C3'-C4'-C5'
9	C	304	FAD	C4B-C5B-O5B-PA
9	C	304	FAD	C5B-O5B-PA-O1A
9	C	304	FAD	C5B-O5B-PA-O2A
9	C	304	FAD	C4'-C5'-O5'-P
8	C	285	F42	C2'-C1'-N10-C10

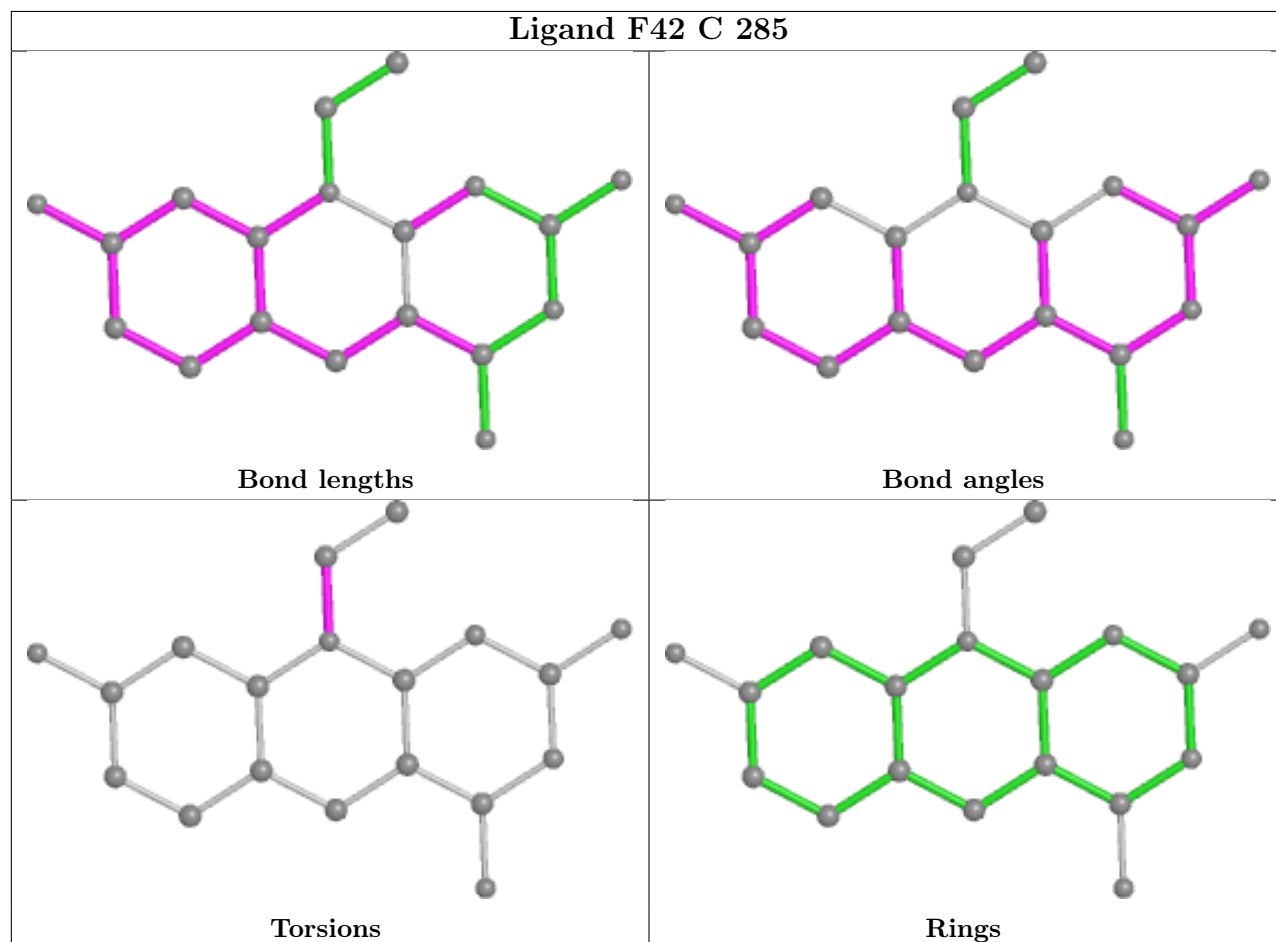
There are no ring outliers.

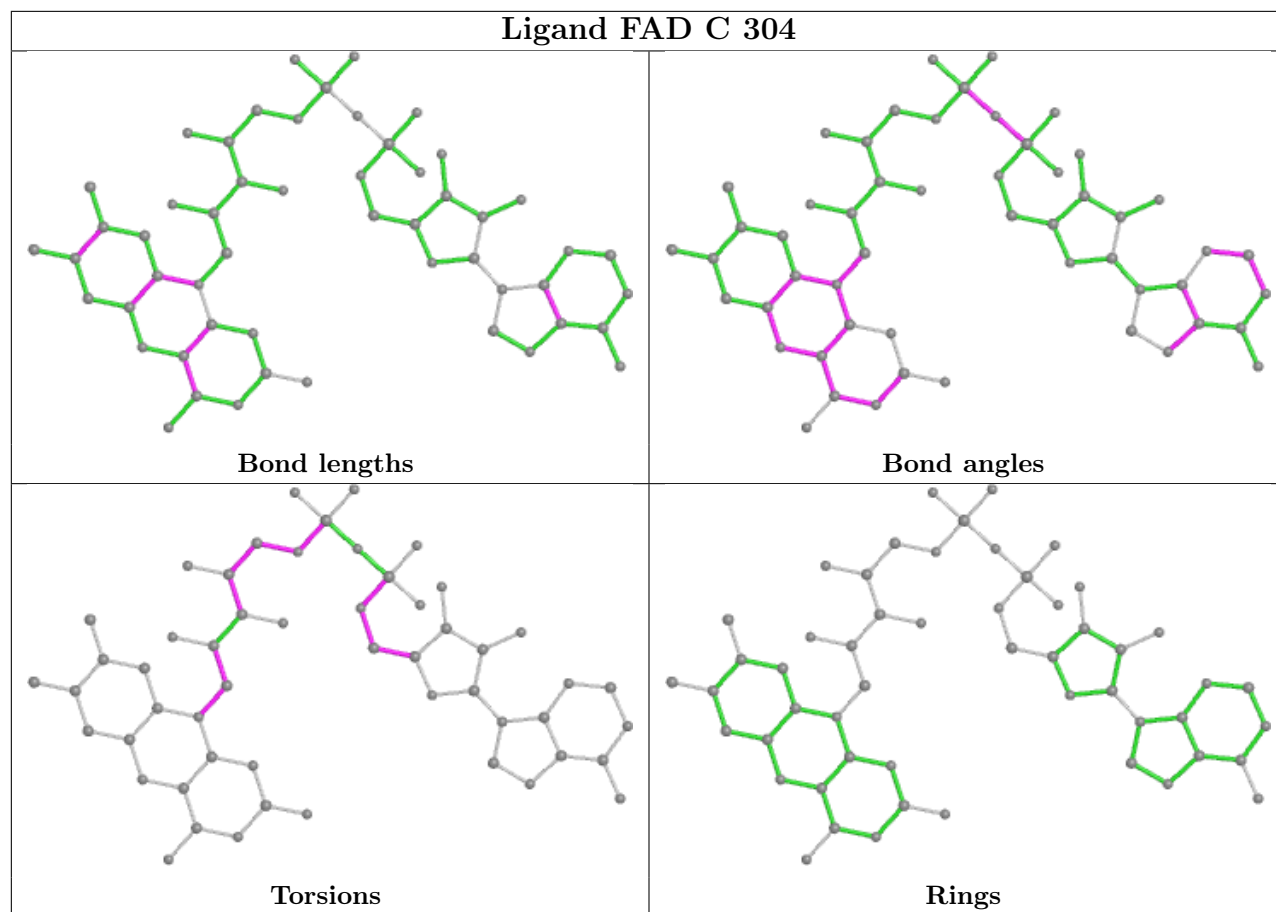
5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	300	SF4	2	0
7	B	302	SF4	1	0
8	C	285	F42	8	0
7	C	303	SF4	3	0
9	C	304	FAD	12	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.