



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:09 pm BST

PDB ID : 5AHS
Title : 3-Sulfinopropionyl-Coenzyme A (3SP-CoA) desulfonase from *Advenella mimgardefordensis* DPN7T: holo crystal structure with the substrate analog succinyl-CoA
Authors : Cianci, M.; Schuermann, M.; Meijers, R.; Schneider, T.R.; Steinbuechel, A.
Deposited on : 2015-02-06
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

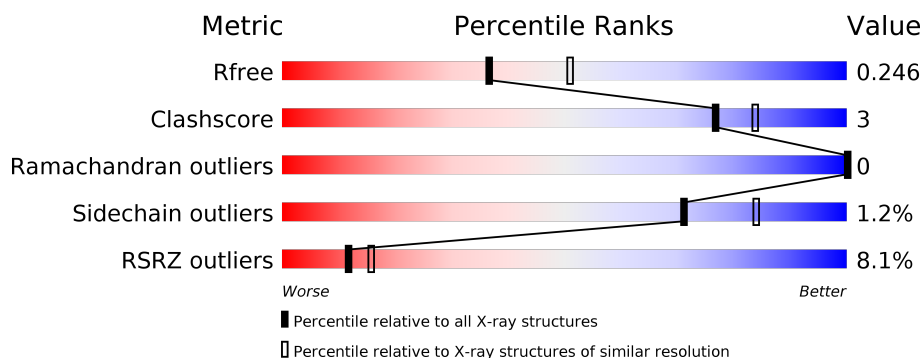
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	401	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div></div> </div> </div>
1	B	401	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div></div> </div> </div>
1	C	401	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> </div>
1	D	401	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div></div> <div></div> </div> </div>
1	E	401	<div> <div>13%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> </div>
1	F	401	<div> <div>18%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div></div> </div> </div>

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
3	COA	A	411	-	-	-	X

2 Entry composition [i](#)

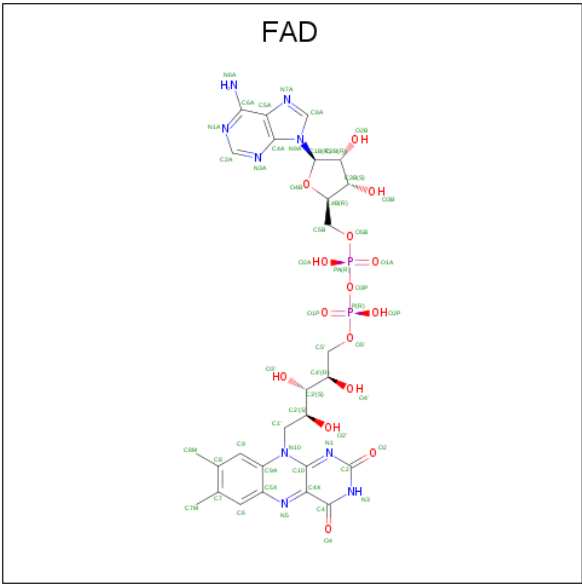
There are 6 unique types of molecules in this entry. The entry contains 19886 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACYL-COA DEHYDROGENASE.

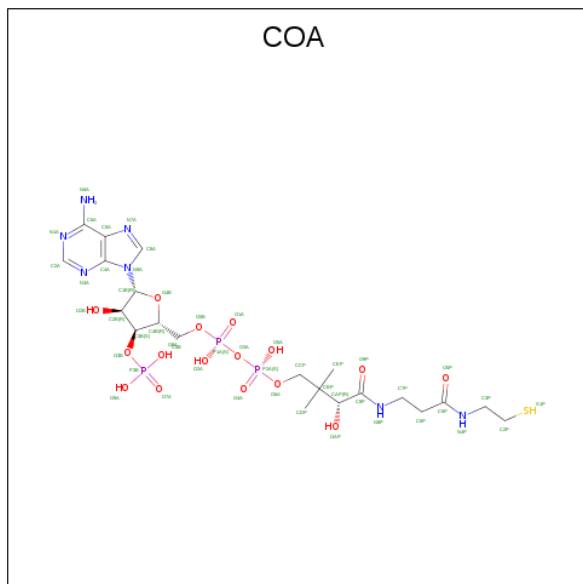
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	1	0
			2980	1871	527	563	19			
1	B	391	Total	C	N	O	S	0	1	0
			2983	1872	528	564	19			
1	C	391	Total	C	N	O	S	0	0	0
			2974	1867	526	562	19			
1	D	390	Total	C	N	O	S	0	0	0
			2962	1858	525	560	19			
1	E	391	Total	C	N	O	S	0	0	0
			2974	1867	526	562	19			
1	F	391	Total	C	N	O	S	0	1	0
			2980	1871	527	563	19			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



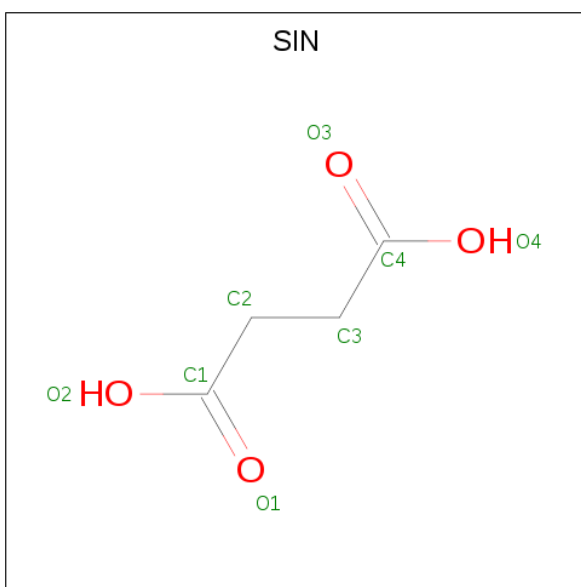
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	E	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	F	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 4 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		

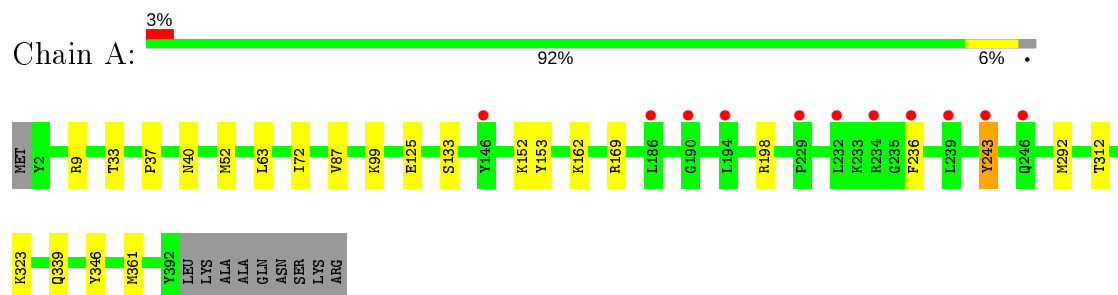
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	327	Total 327	O 327	0	0
6	B	271	Total 271	O 271	0	0
6	C	236	Total 236	O 236	0	0
6	D	220	Total 220	O 220	0	0
6	E	203	Total 203	O 203	0	0
6	F	205	Total 205	O 205	0	0

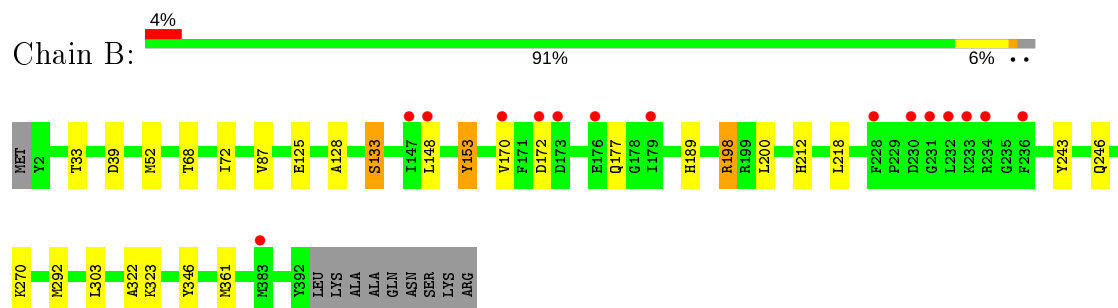
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

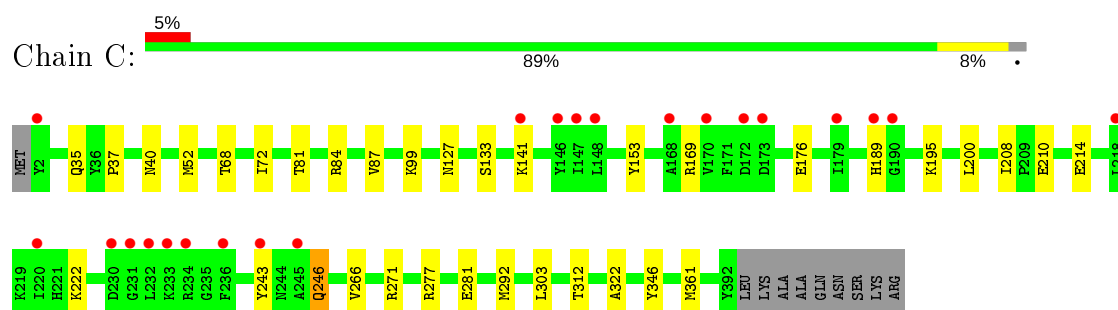
• Molecule 1: ACYL-COA DEHYDROGENASE



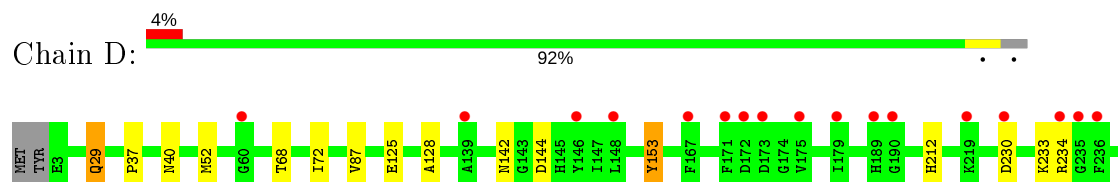
• Molecule 1: ACYL-COA DEHYDROGENASE

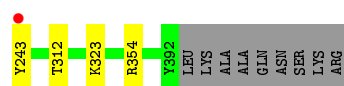


• Molecule 1: ACYL-COA DEHYDROGENASE

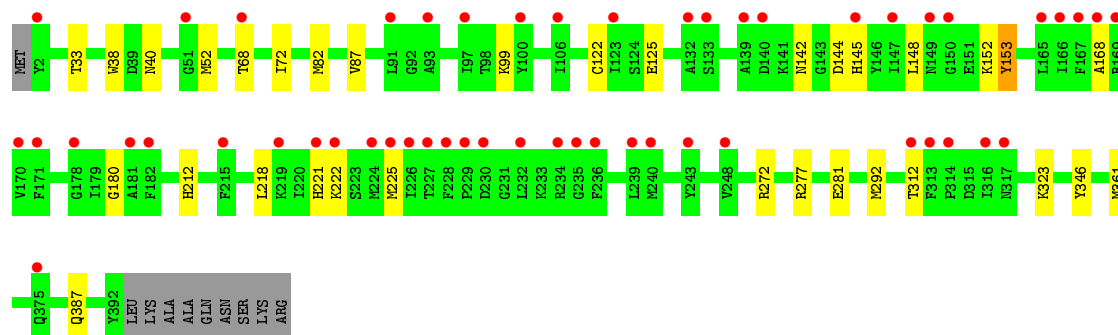
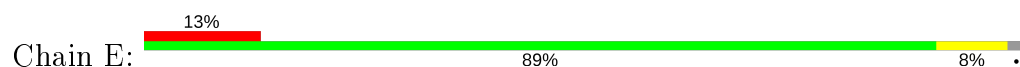


• Molecule 1: ACYL-COA DEHYDROGENASE

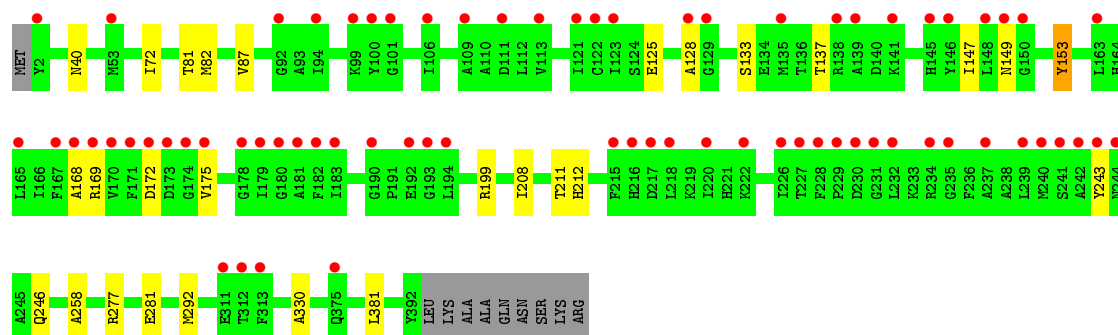
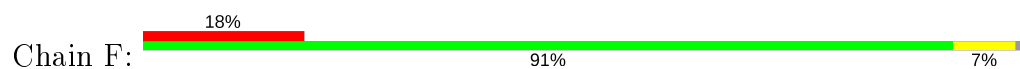




● Molecule 1: ACYL-COA DEHYDROGENASE



● Molecule 1: ACYL-COA DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.07 Å 233.49 Å 121.28 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	116.75 – 2.30 116.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (116.75-2.30) 99.8 (116.75-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.200 , 0.244 0.201 , 0.246	Depositor DCC
R_{free} test set	6352 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19886	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, SO4, FAD, SIN

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	0.21	0/3034	0.36	0/4095
1	B	0.21	0/3034	0.36	0/4095
1	C	0.21	0/3025	0.36	0/4083
1	D	0.21	0/3012	0.36	0/4065
1	E	0.21	0/3025	0.35	0/4083
1	F	0.21	0/3034	0.35	0/4095
All	All	0.21	0/18164	0.36	0/24516

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2980	0	2971	18	0
1	B	2983	0	2970	19	0
1	C	2974	0	2963	22	0
1	D	2962	0	2954	13	0
1	E	2974	0	2963	24	0
1	F	2980	0	2971	14	0
2	A	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	2	0
2	E	53	0	31	1	0
2	F	53	0	31	3	0
3	A	48	0	32	2	0
3	B	48	0	32	1	0
3	D	48	0	32	3	0
3	E	48	0	32	1	0
3	F	48	0	32	2	0
4	C	8	0	4	3	0
5	C	5	0	0	0	0
6	A	327	0	0	6	0
6	B	271	0	0	4	0
6	C	236	0	0	6	0
6	D	220	0	0	4	0
6	E	203	0	0	7	0
6	F	205	0	0	1	0
All	All	19886	0	18142	109	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 3.

All (109) 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:E:122:CYS:SG	6:E:2084:HOH:O	2.44	0.75
1:B:243:TYR:OH	3:B:411:COA:S1P	2.48	0.69
1:E:180:GLY:O	6:E:2105:HOH:O	2.11	0.69
1:A:198:ARG:NH1	6:A:2172:HOH:O	2.29	0.66
1:D:354:ARG:NH1	6:D:2067:HOH:O	2.29	0.66
1:C:271:ARG:NH1	6:C:2160:HOH:O	2.31	0.63
1:A:133:SER:O	1:A:169:ARG:NH2	2.32	0.62
1:B:170:VAL:HG23	1:B:177:GLN:HB2	1.83	0.60
1:A:99:LYS:NZ	6:A:2126:HOH:O	2.34	0.60
4:C:412:SIN:O3	6:C:2188:HOH:O	2.17	0.60
1:A:9:ARG:NH2	6:A:2012:HOH:O	2.31	0.59
1:C:346:TYR:CZ	1:E:361:MET:HB3	2.38	0.59
1:C:246:GLN:NE2	6:C:2151:HOH:O	2.29	0.59
1:B:33:THR:HG22	1:E:33:THR:HG22	1.85	0.59
1:A:236:PHE:O	6:A:2216:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LYS:NZ	1:D:144:ASP:OD2	2.36	0.57
6:C:2162:HOH:O	1:E:387:GLN:O	2.17	0.57
2:A:410:FAD:O2'	3:A:411:COA:S1P	2.61	0.57
1:C:133:SER:O	1:C:169:ARG:NH2	2.38	0.56
1:D:52:MET:HE3	1:D:68:THR:HG22	1.88	0.56
1:C:361:MET:HB3	1:E:346:TYR:CZ	2.41	0.56
1:F:72:ILE:HD13	1:F:87:VAL:HG22	1.88	0.56
1:D:323:LYS:NZ	6:D:2178:HOH:O	2.38	0.56
1:E:142:ASN:ND2	6:E:2097:HOH:O	2.39	0.56
1:A:33:THR:HG22	1:E:38:TRP:HB3	1.87	0.55
1:F:243:TYR:OH	3:F:411:COA:S1P	2.55	0.55
1:C:52:MET:HE3	1:C:68:THR:HG22	1.90	0.54
1:A:361:MET:HB3	1:B:346:TYR:CZ	2.43	0.54
1:F:125:GLU:HB2	1:F:128:ALA:HB3	1.89	0.54
1:C:72:ILE:HD13	1:C:87:VAL:HG22	1.90	0.53
1:D:72:ILE:HD13	1:D:87:VAL:HG22	1.90	0.53
2:E:410:FAD:O2'	3:E:411:COA:S1P	2.66	0.53
2:F:410:FAD:O2A	6:F:2192:HOH:O	2.19	0.53
1:E:72:ILE:HD13	1:E:87:VAL:HG22	1.91	0.53
1:F:137:THR:HG23	1:F:168:ALA:HA	1.90	0.52
1:B:72:ILE:HD13	1:B:87:VAL:HG22	1.91	0.52
1:A:346:TYR:CZ	1:B:361:MET:HB3	2.45	0.52
1:B:125:GLU:HB2	1:B:128:ALA:HB3	1.92	0.51
2:D:410:FAD:HO2'	3:D:411:COA:HS1	1.50	0.51
2:D:410:FAD:O2'	3:D:411:COA:S1P	2.64	0.51
1:A:162:LYS:NZ	6:A:2180:HOH:O	2.42	0.50
1:D:230:ASP:HB2	1:D:234:ARG:HH21	1.76	0.50
2:F:410:FAD:O2'	3:F:411:COA:S1P	2.67	0.50
1:F:277:ARG:HD2	1:F:281:GLU:HB2	1.94	0.49
1:E:168:ALA:N	6:E:2105:HOH:O	2.31	0.49
1:C:81:THR:HG23	1:C:208:ILE:HG13	1.95	0.49
1:E:168:ALA:O	6:E:2105:HOH:O	2.20	0.48
1:C:84:ARG:HE	4:C:412:SIN:C1	2.27	0.48
1:C:127:ASN:HA	1:E:272:ARG:HH12	1.78	0.48
1:A:52:MET:HB3	1:A:63:LEU:HD12	1.96	0.47
1:B:148:LEU:HB2	1:B:218:LEU:HB3	1.96	0.47
1:C:277:ARG:HD2	1:C:281:GLU:HB2	1.96	0.47
1:A:323:LYS:NZ	6:A:2271:HOH:O	2.47	0.47
1:E:292:MET:HE3	1:E:292:MET:HB2	1.74	0.46
1:B:323:LYS:NZ	6:B:2226:HOH:O	2.47	0.46
1:D:37:PRO:HB2	1:D:40:ASN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:GLY:N	6:E:2105:HOH:O	2.49	0.46
1:D:153:TYR:HA	1:D:212:HIS:HA	1.98	0.46
1:E:52:MET:HE3	1:E:68:THR:HG22	1.98	0.46
1:D:142:ASN:ND2	6:D:2110:HOH:O	2.49	0.45
1:B:198:ARG:NH1	6:B:2157:HOH:O	2.49	0.45
1:C:141:LYS:NZ	6:C:2102:HOH:O	2.48	0.45
1:B:52:MET:HE3	1:B:68:THR:HG22	1.99	0.45
1:D:243:TYR:OH	3:D:411:COA:S1P	2.56	0.45
1:E:144:ASP:HA	1:E:222:LYS:NZ	2.32	0.45
1:B:246[A]:GLN:NE2	6:B:2171:HOH:O	2.48	0.44
1:E:323:LYS:NZ	6:E:2163:HOH:O	2.51	0.44
1:E:40:ASN:HB3	1:E:82:MET:SD	2.57	0.44
1:F:81:THR:HG23	1:F:208:ILE:HG13	2.00	0.44
1:D:125:GLU:HB2	1:D:128:ALA:HB3	1.99	0.44
1:A:37:PRO:HB2	1:A:40:ASN:HB2	2.00	0.43
1:C:37:PRO:HB2	1:C:40:ASN:HB2	1.99	0.43
1:E:148:LEU:HB2	1:E:218:LEU:HB3	2.01	0.43
1:F:292:MET:HB2	1:F:292:MET:HE3	1.84	0.43
1:C:292:MET:HE3	1:C:292:MET:HB2	1.82	0.43
1:E:277:ARG:HD2	1:E:281:GLU:HB2	2.00	0.43
1:E:125:GLU:HG2	1:E:152:LYS:HD3	2.01	0.43
1:E:153:TYR:HA	1:E:212:HIS:HA	2.01	0.43
1:A:339:GLN:O	2:B:410:FAD:O3B	2.30	0.43
1:C:84:ARG:HH21	4:C:412:SIN:H32	1.83	0.43
1:A:243:TYR:OH	3:A:411:COA:S1P	2.59	0.43
1:B:153:TYR:HA	1:B:212:HIS:HA	2.01	0.43
1:C:169:ARG:NH1	1:C:176:GLU:OE2	2.48	0.42
2:F:410:FAD:O5'	2:F:410:FAD:O3'	2.36	0.42
1:C:303:LEU:HD23	1:C:322:ALA:HB1	1.99	0.42
1:F:258:ALA:HB2	1:F:330:ALA:HA	2.01	0.42
1:B:292:MET:HE3	1:B:292:MET:HB2	1.83	0.42
1:A:125:GLU:HG2	1:A:152:LYS:HD3	2.01	0.42
1:F:40:ASN:HB3	1:F:82:MET:SD	2.60	0.42
1:F:153:TYR:HA	1:F:212:HIS:HA	2.01	0.42
1:A:292:MET:HE3	1:A:292:MET:HB2	1.89	0.42
1:C:195:LYS:HB3	1:C:214:GLU:HB2	2.02	0.42
1:D:233:LYS:NZ	6:D:2122:HOH:O	2.52	0.42
1:C:99:LYS:HD3	1:C:312:THR:HG21	2.02	0.41
1:D:29:GLN:HA	1:D:29:GLN:HE21	1.85	0.41
1:E:145:HIS:CD2	1:E:221:HIS:HD2	2.38	0.41
1:C:200:LEU:N	1:C:210:GLU:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LYS:HD3	1:A:312:THR:HG21	2.03	0.41
1:A:72:ILE:HD13	1:A:87:VAL:HG22	2.01	0.41
1:F:199:ARG:HA	1:F:211:THR:HG22	2.03	0.41
1:B:133:SER:OG	6:B:2138:HOH:O	2.21	0.41
1:F:133:SER:O	1:F:169:ARG:NH2	2.55	0.40
1:F:172:ASP:O	1:F:175:VAL:HG12	2.20	0.40
1:B:303:LEU:HD23	1:B:322:ALA:HB1	2.03	0.40
1:E:99:LYS:HD3	1:E:312:THR:HG21	2.02	0.40
1:B:200:LEU:HD21	1:B:212:HIS:HE1	1.85	0.40
1:C:35:GLN:NE2	6:C:2029:HOH:O	2.41	0.40
1:B:39:ASP:N	1:B:39:ASP:OD1	2.55	0.40
1:C:266:VAL:HG13	1:F:381:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	390/401 (97%)	382 (98%)	8 (2%)	0	100	100
1	B	390/401 (97%)	380 (97%)	10 (3%)	0	100	100
1	C	389/401 (97%)	381 (98%)	8 (2%)	0	100	100
1	D	388/401 (97%)	380 (98%)	8 (2%)	0	100	100
1	E	389/401 (97%)	381 (98%)	8 (2%)	0	100	100
1	F	390/401 (97%)	377 (97%)	13 (3%)	0	100	100
All	All	2336/2406 (97%)	2281 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	304/311 (98%)	302 (99%)	2 (1%)	84	92
1	B	304/311 (98%)	299 (98%)	5 (2%)	62	78
1	C	303/311 (97%)	298 (98%)	5 (2%)	60	76
1	D	302/311 (97%)	299 (99%)	3 (1%)	76	87
1	E	303/311 (97%)	301 (99%)	2 (1%)	84	92
1	F	304/311 (98%)	299 (98%)	5 (2%)	62	78
All	All	1820/1866 (98%)	1798 (99%)	22 (1%)	71	84

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	TYR
1	A	243	TYR
1	B	133	SER
1	B	153	TYR
1	B	172	ASP
1	B	189	HIS
1	B	198	ARG
1	C	153	TYR
1	C	189	HIS
1	C	222	LYS
1	C	243	TYR
1	C	246	GLN
1	D	29	GLN
1	D	153	TYR
1	D	312	THR
1	E	153	TYR
1	E	225	MET
1	F	147	ILE
1	F	149	ASN
1	F	153	TYR
1	F	246[A]	GLN
1	F	246[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	212	HIS
1	D	29	GLN
1	D	212	HIS
1	D	295	GLN
1	D	355	HIS
1	D	370	GLN
1	E	212	HIS
1	F	177	GLN
1	F	212	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
3	COA	A	411	-	41,50,50	0.81	1 (2%)	52,75,75	1.13	3 (5%)
3	COA	D	411	-	41,50,50	0.81	1 (2%)	52,75,75	1.17	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	COA	B	411	-	41,50,50	0.80	1 (2%)	52,75,75	1.17	3 (5%)
4	SIN	C	412	-	1,7,7	0.15	0	2,8,8	2.45	2 (100%)
2	FAD	F	410	-	51,58,58	1.87	6 (11%)	60,89,89	1.96	12 (20%)
2	FAD	D	410	-	51,58,58	1.85	6 (11%)	60,89,89	1.89	12 (20%)
2	FAD	B	410	-	51,58,58	1.85	6 (11%)	60,89,89	1.89	10 (16%)
2	FAD	E	410	-	51,58,58	1.86	6 (11%)	60,89,89	1.92	13 (21%)
2	FAD	C	410	-	51,58,58	1.83	6 (11%)	60,89,89	1.92	11 (18%)
3	COA	E	411	-	41,50,50	0.80	1 (2%)	52,75,75	1.15	5 (9%)
2	FAD	A	410	-	51,58,58	1.82	6 (11%)	60,89,89	1.89	11 (18%)
5	SO4	C	1393	-	4,4,4	0.30	0	6,6,6	0.76	0
3	COA	F	411	-	41,50,50	0.80	1 (2%)	52,75,75	1.05	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	A	411	-	-	9/44/64/64	0/3/3/3
3	COA	D	411	-	-	5/44/64/64	0/3/3/3
3	COA	B	411	-	-	10/44/64/64	0/3/3/3
4	SIN	C	412	-	-	0/1/5/5	-
2	FAD	F	410	-	-	7/30/50/50	0/6/6/6
2	FAD	D	410	-	-	11/30/50/50	0/6/6/6
2	FAD	B	410	-	-	8/30/50/50	0/6/6/6
2	FAD	E	410	-	-	8/30/50/50	0/6/6/6
2	FAD	C	410	-	-	11/30/50/50	0/6/6/6
3	COA	E	411	-	-	10/44/64/64	0/3/3/3
2	FAD	A	410	-	-	10/30/50/50	0/6/6/6
3	COA	F	411	-	-	13/44/64/64	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	410	FAD	C4X-C10	9.69	1.48	1.38
2	D	410	FAD	C4X-C10	9.64	1.48	1.38
2	E	410	FAD	C4X-C10	9.59	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	410	FAD	C4X-C10	9.53	1.48	1.38
2	B	410	FAD	C4X-C10	9.51	1.48	1.38
2	A	410	FAD	C4X-C10	9.38	1.48	1.38
2	E	410	FAD	C4-C4X	4.39	1.48	1.41
2	F	410	FAD	C4-C4X	4.37	1.48	1.41
2	B	410	FAD	C4-C4X	4.32	1.48	1.41
2	D	410	FAD	C4-C4X	4.21	1.48	1.41
2	C	410	FAD	C4-C4X	4.17	1.48	1.41
2	A	410	FAD	C4-C4X	4.13	1.48	1.41
2	A	410	FAD	C9A-C5X	3.55	1.49	1.42
2	E	410	FAD	C9A-C5X	3.54	1.49	1.42
2	F	410	FAD	C9A-C5X	3.54	1.49	1.42
2	B	410	FAD	C9A-C5X	3.52	1.49	1.42
2	D	410	FAD	C9A-C5X	3.51	1.49	1.42
2	C	410	FAD	C9A-C5X	3.50	1.49	1.42
2	F	410	FAD	C8-C7	3.30	1.49	1.40
2	E	410	FAD	C8-C7	3.27	1.49	1.40
2	A	410	FAD	C8-C7	3.26	1.49	1.40
2	B	410	FAD	C8-C7	3.25	1.49	1.40
2	D	410	FAD	C8-C7	3.23	1.49	1.40
2	C	410	FAD	C8-C7	3.23	1.48	1.40
3	A	411	COA	C5A-C4A	2.48	1.47	1.40
3	E	411	COA	C5A-C4A	2.48	1.47	1.40
2	D	410	FAD	C5A-C4A	2.47	1.47	1.40
3	B	411	COA	C5A-C4A	2.46	1.47	1.40
2	B	410	FAD	C5A-C4A	2.46	1.47	1.40
2	F	410	FAD	C5A-C4A	2.45	1.47	1.40
3	F	411	COA	C5A-C4A	2.45	1.47	1.40
2	E	410	FAD	C5A-C4A	2.45	1.47	1.40
3	D	411	COA	C5A-C4A	2.44	1.47	1.40
2	A	410	FAD	C5A-C4A	2.44	1.47	1.40
2	B	410	FAD	C9A-N10	2.40	1.41	1.38
2	C	410	FAD	C5A-C4A	2.40	1.47	1.40
2	E	410	FAD	C9A-N10	2.35	1.41	1.38
2	D	410	FAD	C9A-N10	2.34	1.41	1.38
2	F	410	FAD	C9A-N10	2.31	1.41	1.38
2	A	410	FAD	C9A-N10	2.27	1.41	1.38
2	C	410	FAD	C9A-N10	2.19	1.41	1.38

All (88) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	410	FAD	C4-N3-C2	8.44	122.26	115.14
2	B	410	FAD	C4-N3-C2	8.38	122.22	115.14
2	E	410	FAD	C4-N3-C2	8.34	122.19	115.14
2	C	410	FAD	C4-N3-C2	8.33	122.17	115.14
2	A	410	FAD	C4-N3-C2	8.26	122.12	115.14
2	D	410	FAD	C4-N3-C2	8.22	122.08	115.14
2	F	410	FAD	C4-C4X-C10	-5.21	116.50	119.95
2	C	410	FAD	C4-C4X-C10	-4.92	116.69	119.95
2	E	410	FAD	C4-C4X-C10	-4.70	116.84	119.95
2	B	410	FAD	C4-C4X-C10	-4.62	116.89	119.95
2	A	410	FAD	C4-C4X-C10	-4.58	116.92	119.95
2	D	410	FAD	C4-C4X-C10	-4.57	116.93	119.95
2	A	410	FAD	C1'-N10-C9A	4.31	121.69	118.29
2	E	410	FAD	C4X-N5-C5X	4.22	120.99	116.77
2	F	410	FAD	C4X-N5-C5X	4.13	120.90	116.77
2	B	410	FAD	C4X-N5-C5X	4.12	120.88	116.77
2	C	410	FAD	C1'-N10-C9A	4.11	121.53	118.29
2	D	410	FAD	C4X-N5-C5X	4.04	120.81	116.77
2	F	410	FAD	C1'-N10-C9A	4.02	121.45	118.29
2	C	410	FAD	C4X-N5-C5X	4.00	120.77	116.77
2	B	410	FAD	C1'-N10-C9A	3.92	121.38	118.29
2	A	410	FAD	C4X-N5-C5X	3.90	120.67	116.77
3	B	411	COA	P2A-O3A-P1A	-3.82	119.72	132.83
2	E	410	FAD	C1'-N10-C9A	3.80	121.29	118.29
2	D	410	FAD	C1'-N10-C9A	3.77	121.26	118.29
3	D	411	COA	P2A-O3A-P1A	-3.73	120.01	132.83
2	C	410	FAD	C4X-C4-N3	-3.68	118.40	123.43
2	A	410	FAD	C4X-C4-N3	-3.67	118.42	123.43
2	B	410	FAD	C4X-C4-N3	-3.64	118.45	123.43
2	E	410	FAD	C4X-C4-N3	-3.63	118.46	123.43
2	D	410	FAD	C4X-C4-N3	-3.63	118.47	123.43
3	A	411	COA	P2A-O3A-P1A	-3.62	120.39	132.83
2	F	410	FAD	C4X-C4-N3	-3.58	118.53	123.43
2	F	410	FAD	C4-C4X-N5	3.36	122.44	118.60
2	E	410	FAD	P-O3P-PA	-3.35	121.33	132.83
2	F	410	FAD	P-O3P-PA	-3.25	121.67	132.83
3	F	411	COA	N3A-C2A-N1A	-3.25	123.61	128.68
3	B	411	COA	N3A-C2A-N1A	-3.24	123.61	128.68
2	B	410	FAD	N3A-C2A-N1A	-3.22	123.64	128.68
2	C	410	FAD	N3A-C2A-N1A	-3.22	123.64	128.68
3	A	411	COA	N3A-C2A-N1A	-3.22	123.65	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	410	FAD	N3A-C2A-N1A	-3.22	123.65	128.68
2	E	410	FAD	N3A-C2A-N1A	-3.21	123.66	128.68
3	D	411	COA	N3A-C2A-N1A	-3.21	123.67	128.68
3	E	411	COA	N3A-C2A-N1A	-3.19	123.69	128.68
2	D	410	FAD	N3A-C2A-N1A	-3.19	123.70	128.68
2	A	410	FAD	N3A-C2A-N1A	-3.17	123.73	128.68
2	D	410	FAD	P-O3P-PA	-3.05	122.35	132.83
2	C	410	FAD	C4-C4X-N5	3.05	122.08	118.60
2	C	410	FAD	P-O3P-PA	-3.03	122.42	132.83
2	E	410	FAD	C4-C4X-N5	2.97	121.99	118.60
3	E	411	COA	P2A-O3A-P1A	-2.97	122.64	132.83
2	B	410	FAD	C4-C4X-N5	2.94	121.95	118.60
2	A	410	FAD	P-O3P-PA	-2.84	123.09	132.83
2	B	410	FAD	P-O3P-PA	-2.82	123.16	132.83
2	D	410	FAD	C9A-N10-C10	-2.76	118.29	121.91
2	A	410	FAD	C9A-N10-C10	-2.76	118.30	121.91
2	D	410	FAD	C4-C4X-N5	2.74	121.73	118.60
3	E	411	COA	C4A-C5A-N7A	-2.74	106.55	109.40
3	F	411	COA	C4A-C5A-N7A	-2.73	106.56	109.40
2	A	410	FAD	C4-C4X-N5	2.70	121.69	118.60
2	A	410	FAD	C4A-C5A-N7A	-2.70	106.59	109.40
3	B	411	COA	C4A-C5A-N7A	-2.69	106.59	109.40
2	B	410	FAD	C4A-C5A-N7A	-2.68	106.60	109.40
2	C	410	FAD	C9A-N10-C10	-2.66	118.42	121.91
2	F	410	FAD	C9A-N10-C10	-2.66	118.43	121.91
2	D	410	FAD	C4A-C5A-N7A	-2.64	106.65	109.40
3	A	411	COA	C4A-C5A-N7A	-2.63	106.65	109.40
2	E	410	FAD	C9A-N10-C10	-2.63	118.46	121.91
2	F	410	FAD	C4A-C5A-N7A	-2.61	106.67	109.40
2	B	410	FAD	C9A-N10-C10	-2.59	118.51	121.91
2	C	410	FAD	C4A-C5A-N7A	-2.59	106.70	109.40
2	E	410	FAD	C4A-C5A-N7A	-2.59	106.70	109.40
3	D	411	COA	C4A-C5A-N7A	-2.55	106.74	109.40
4	C	412	SIN	C2-C3-C4	-2.54	108.40	112.67
2	D	410	FAD	C5X-C9A-N10	2.42	119.47	117.72
4	C	412	SIN	C3-C2-C1	-2.36	108.72	112.67
2	D	410	FAD	C1'-N10-C10	2.27	120.44	118.41
2	F	410	FAD	C5X-C9A-N10	2.27	119.36	117.72
2	C	410	FAD	C5X-C9A-N10	2.26	119.35	117.72
2	A	410	FAD	C5X-C9A-N10	2.24	119.34	117.72
2	E	410	FAD	C3B-C2B-C1B	2.18	104.27	100.98
2	E	410	FAD	C5X-C9A-N10	2.16	119.28	117.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	411	COA	O6A-CCP-CBP	-2.11	107.16	110.55
2	F	410	FAD	C3B-C2B-C1B	2.09	104.13	100.98
3	E	411	COA	C3B-C2B-C1B	2.07	104.47	99.89
2	E	410	FAD	C1'-N10-C10	2.06	120.25	118.41
3	D	411	COA	C7P-C6P-C5P	-2.05	108.94	112.36

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	411	COA	CCP-O6A-P2A-O3A
3	A	411	COA	CAP-C9P-N8P-C7P
3	A	411	COA	S1P-C2P-C3P-N4P
3	D	411	COA	O4B-C4B-C5B-O5B
3	D	411	COA	CCP-O6A-P2A-O3A
3	B	411	COA	C5B-O5B-P1A-O1A
3	B	411	COA	CCP-O6A-P2A-O4A
3	B	411	COA	S1P-C2P-C3P-N4P
2	F	410	FAD	C5B-O5B-PA-O2A
2	F	410	FAD	C2'-C3'-C4'-O4'
2	F	410	FAD	C2'-C3'-C4'-C5'
2	F	410	FAD	O3'-C3'-C4'-O4'
2	F	410	FAD	O3'-C3'-C4'-C5'
2	D	410	FAD	C5B-O5B-PA-O2A
2	D	410	FAD	C1'-C2'-C3'-C4'
2	D	410	FAD	C2'-C3'-C4'-O4'
2	D	410	FAD	C2'-C3'-C4'-C5'
2	D	410	FAD	O3'-C3'-C4'-O4'
2	D	410	FAD	O3'-C3'-C4'-C5'
2	B	410	FAD	C5B-O5B-PA-O2A
2	B	410	FAD	C2'-C3'-C4'-O4'
2	B	410	FAD	C2'-C3'-C4'-C5'
2	B	410	FAD	O3'-C3'-C4'-O4'
2	B	410	FAD	O3'-C3'-C4'-C5'
2	E	410	FAD	C5B-O5B-PA-O2A
2	C	410	FAD	C5B-O5B-PA-O2A
2	C	410	FAD	C1'-C2'-C3'-C4'
2	C	410	FAD	C2'-C3'-C4'-O4'
2	C	410	FAD	O3'-C3'-C4'-O4'
2	C	410	FAD	O3'-C3'-C4'-C5'
3	E	411	COA	C3B-O3B-P3B-O9A
3	E	411	COA	C5B-O5B-P1A-O2A

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Mol	Chain	Res	Type	Atoms
3	E	411	COA	CCP-O6A-P2A-O3A
3	E	411	COA	CCP-O6A-P2A-O4A
3	E	411	COA	CCP-O6A-P2A-O5A
2	A	410	FAD	C5B-O5B-PA-O2A
2	A	410	FAD	C2'-C3'-C4'-O4'
2	A	410	FAD	O3'-C3'-C4'-O4'
2	A	410	FAD	O3'-C3'-C4'-C5'
3	F	411	COA	C5B-O5B-P1A-O1A
3	F	411	COA	CCP-O6A-P2A-O3A
3	F	411	COA	CAP-CBP-CCP-O6A
3	A	411	COA	O9P-C9P-N8P-C7P
3	A	411	COA	O4B-C4B-C5B-O5B
3	F	411	COA	O4B-C4B-C5B-O5B
2	C	410	FAD	C2'-C3'-C4'-C5'
2	A	410	FAD	C2'-C3'-C4'-C5'
3	F	411	COA	CDP-CBP-CCP-O6A
3	F	411	COA	CEP-CBP-CCP-O6A
2	C	410	FAD	O2'-C2'-C3'-O3'
2	C	410	FAD	O2'-C2'-C3'-C4'
3	B	411	COA	O4B-C4B-C5B-O5B
2	E	410	FAD	O3'-C3'-C4'-C5'
3	B	411	COA	P1A-O3A-P2A-O6A
3	F	411	COA	P1A-O3A-P2A-O6A
3	A	411	COA	C3B-O3B-P3B-O8A
3	A	411	COA	C3B-O3B-P3B-O9A
3	B	411	COA	C5B-O5B-P1A-O3A
3	B	411	COA	CCP-O6A-P2A-O3A
2	F	410	FAD	C5B-O5B-PA-O3P
2	D	410	FAD	C5B-O5B-PA-O3P
2	B	410	FAD	C5B-O5B-PA-O3P
2	E	410	FAD	C5B-O5B-PA-O3P
2	C	410	FAD	C5B-O5B-PA-O3P
3	E	411	COA	C5B-O5B-P1A-O3A
2	A	410	FAD	C5B-O5B-PA-O3P
3	F	411	COA	C3B-O3B-P3B-O9A
2	E	410	FAD	O3'-C3'-C4'-O4'
3	E	411	COA	P1A-O3A-P2A-O4A
2	E	410	FAD	C2'-C3'-C4'-C5'
2	D	410	FAD	O2'-C2'-C3'-C4'
2	E	410	FAD	C2'-C3'-C4'-O4'
3	A	411	COA	CCP-O6A-P2A-O4A
3	D	411	COA	CCP-O6A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
3	B	411	COA	C5B-O5B-P1A-O2A
2	F	410	FAD	C5B-O5B-PA-O1A
2	B	410	FAD	C5B-O5B-PA-O1A
2	E	410	FAD	C5B-O5B-PA-O1A
2	C	410	FAD	C5B-O5B-PA-O1A
3	E	411	COA	C5B-O5B-P1A-O1A
3	F	411	COA	C5B-O5B-P1A-O2A
3	F	411	COA	CCP-O6A-P2A-O4A
2	C	410	FAD	C1'-C2'-C3'-O3'
2	D	410	FAD	O2'-C2'-C3'-O3'
3	B	411	COA	C3B-C4B-C5B-O5B
3	F	411	COA	C2P-C3P-N4P-C5P
3	E	411	COA	P1A-O3A-P2A-O5A
3	B	411	COA	C4B-C5B-O5B-P1A
3	D	411	COA	C2P-C3P-N4P-C5P
3	D	411	COA	C3B-C4B-C5B-O5B
3	F	411	COA	C3B-O3B-P3B-O8A
3	F	411	COA	C5B-O5B-P1A-O3A
3	A	411	COA	P1A-O3A-P2A-O5A
2	B	410	FAD	PA-O3P-P-O2P
2	A	410	FAD	PA-O3P-P-O2P
2	D	410	FAD	C5B-O5B-PA-O1A
2	A	410	FAD	C5B-O5B-PA-O1A
3	E	411	COA	O4B-C4B-C5B-O5B
2	D	410	FAD	C1'-C2'-C3'-O3'
2	E	410	FAD	C1'-C2'-C3'-O3'
2	A	410	FAD	C1'-C2'-C3'-O3'
2	A	410	FAD	O2'-C2'-C3'-O3'

There are no ring outliers.

11 monomers are involved in 15 short contacts:

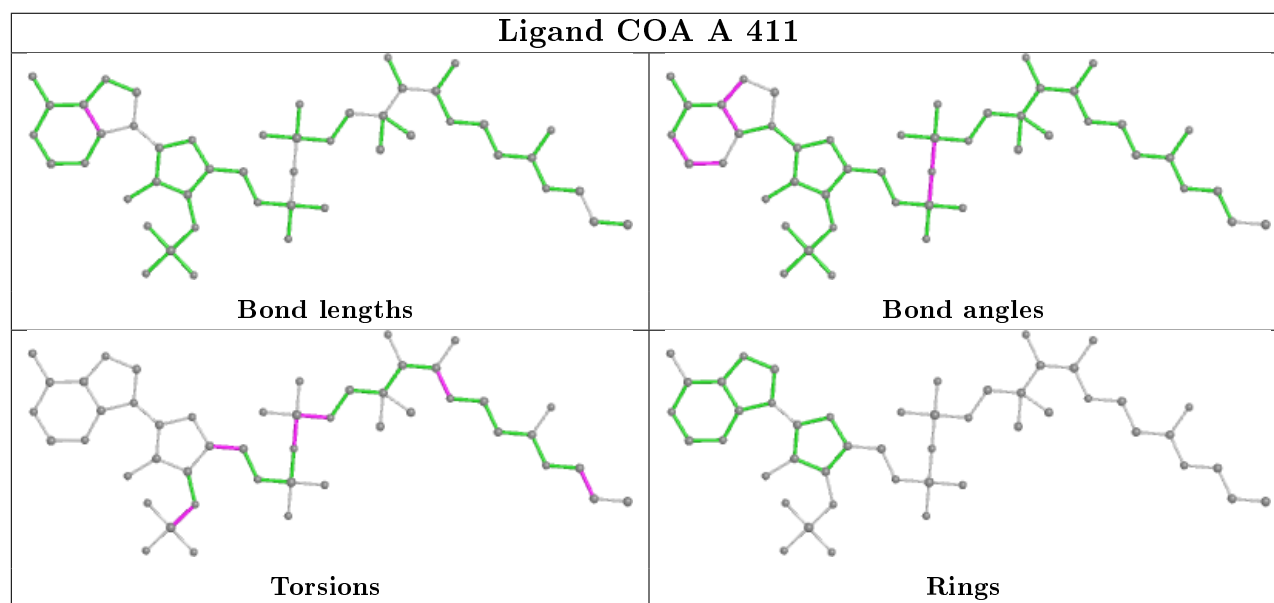
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	411	COA	2	0
3	D	411	COA	3	0
3	B	411	COA	1	0
4	C	412	SIN	3	0
2	F	410	FAD	3	0
2	D	410	FAD	2	0
2	B	410	FAD	1	0
2	E	410	FAD	1	0
3	E	411	COA	1	0

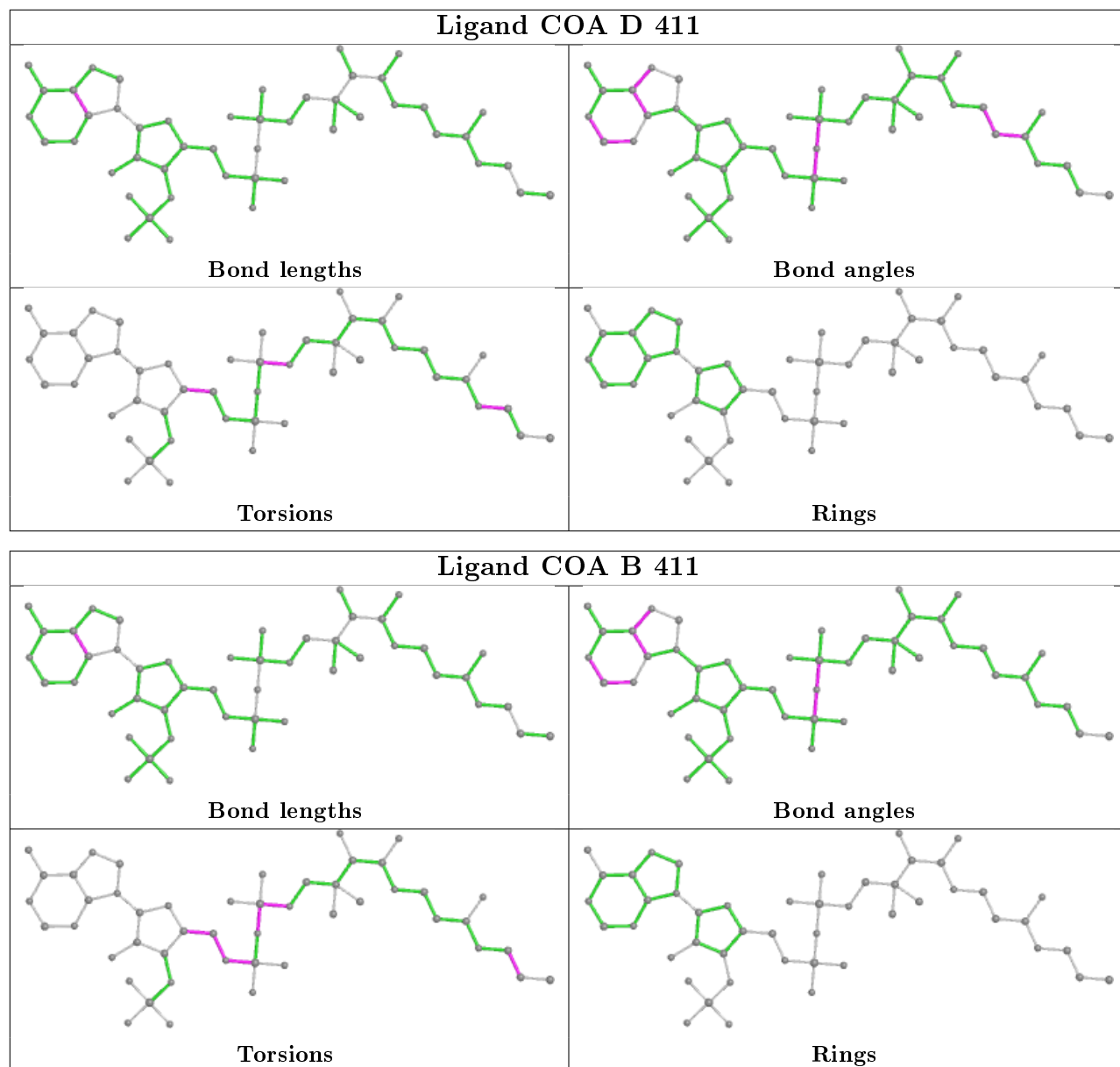
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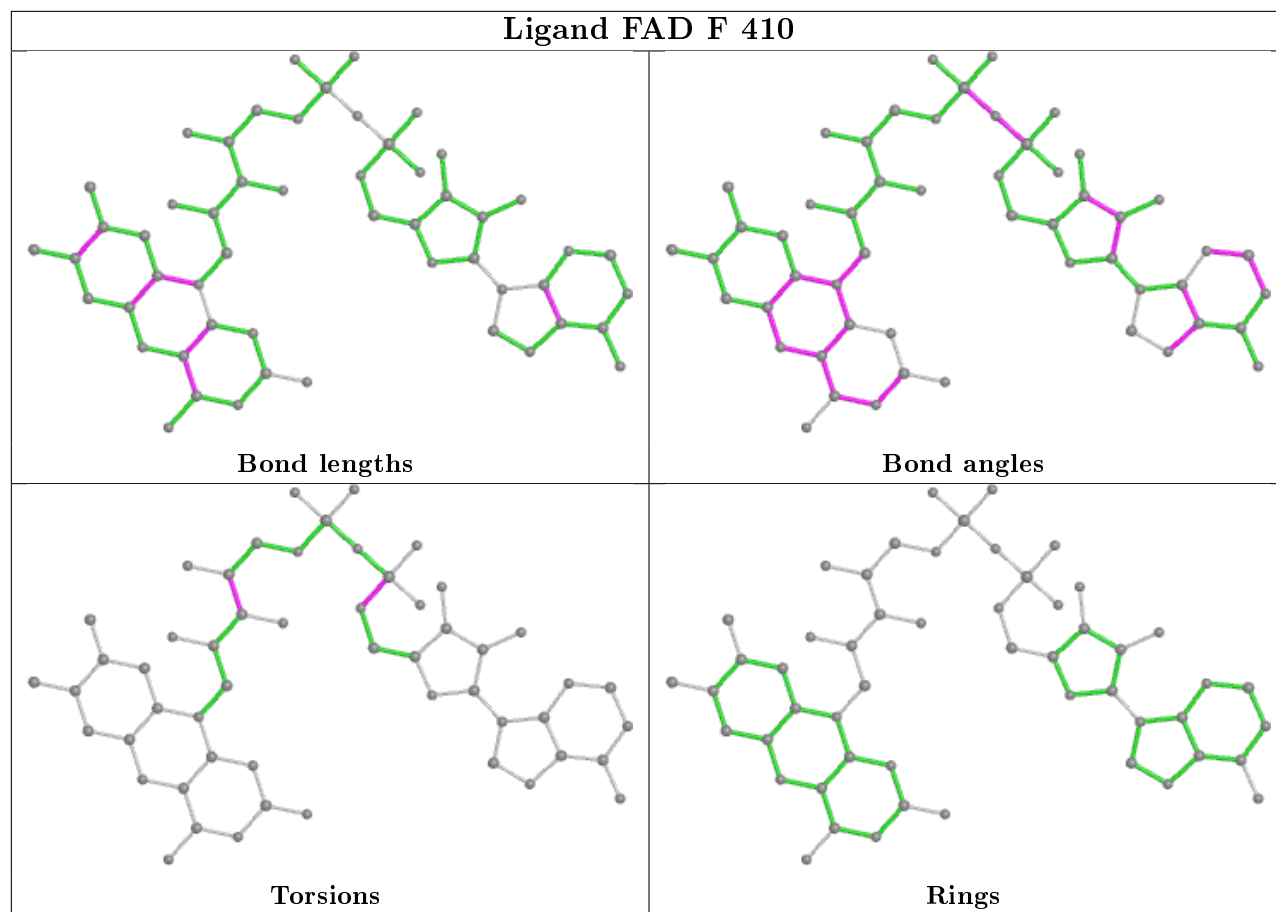
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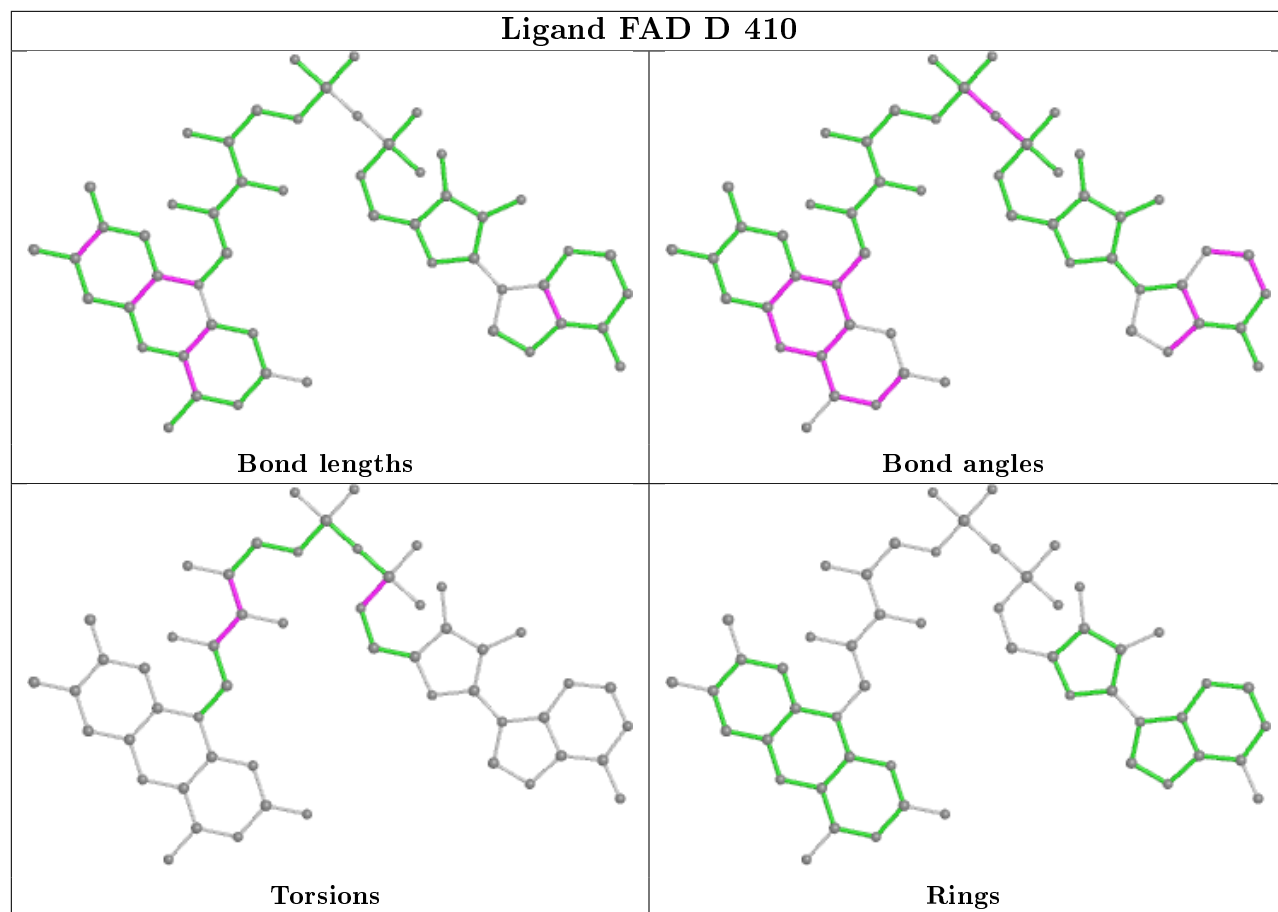
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	410	FAD	1	0
3	F	411	COA	2	0

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.

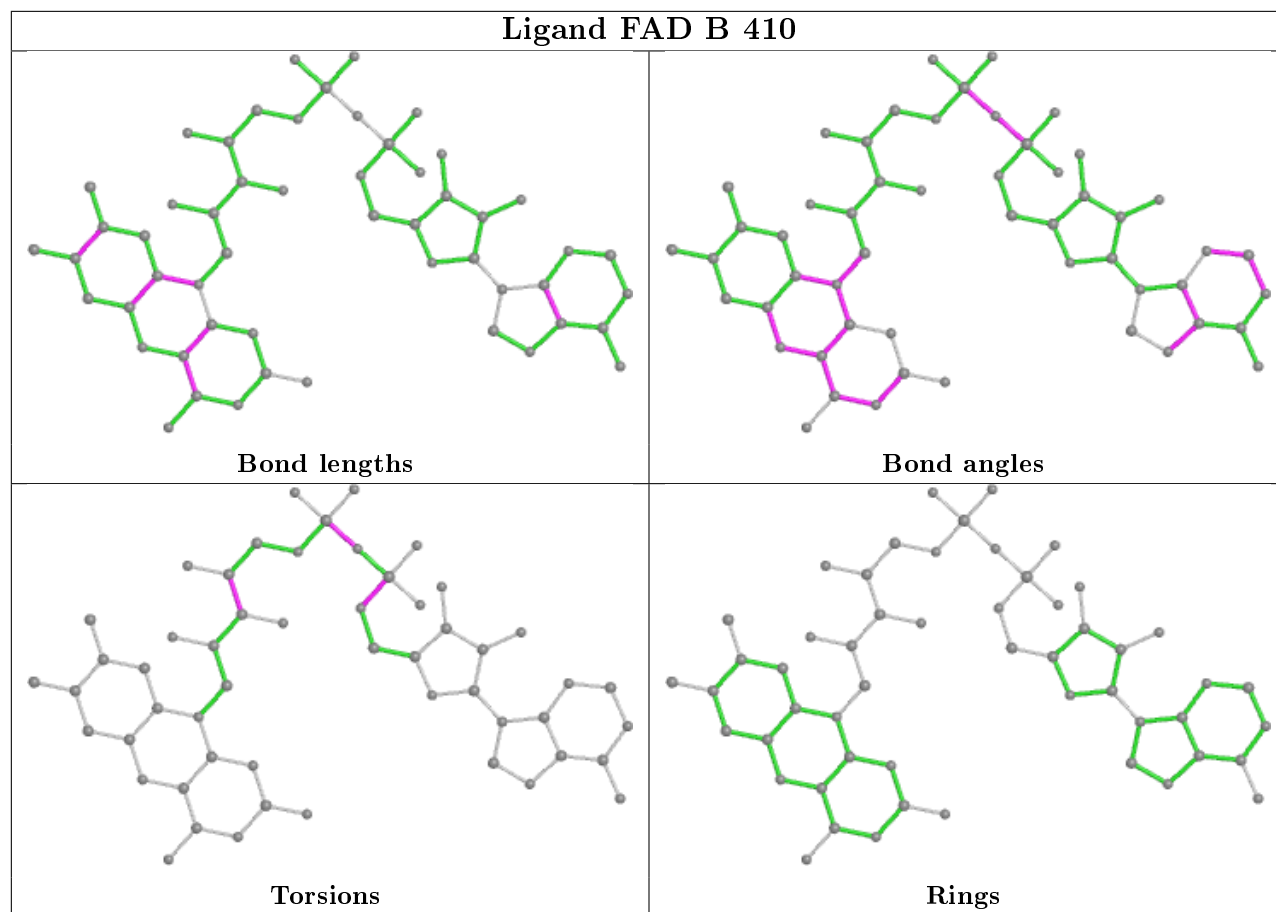


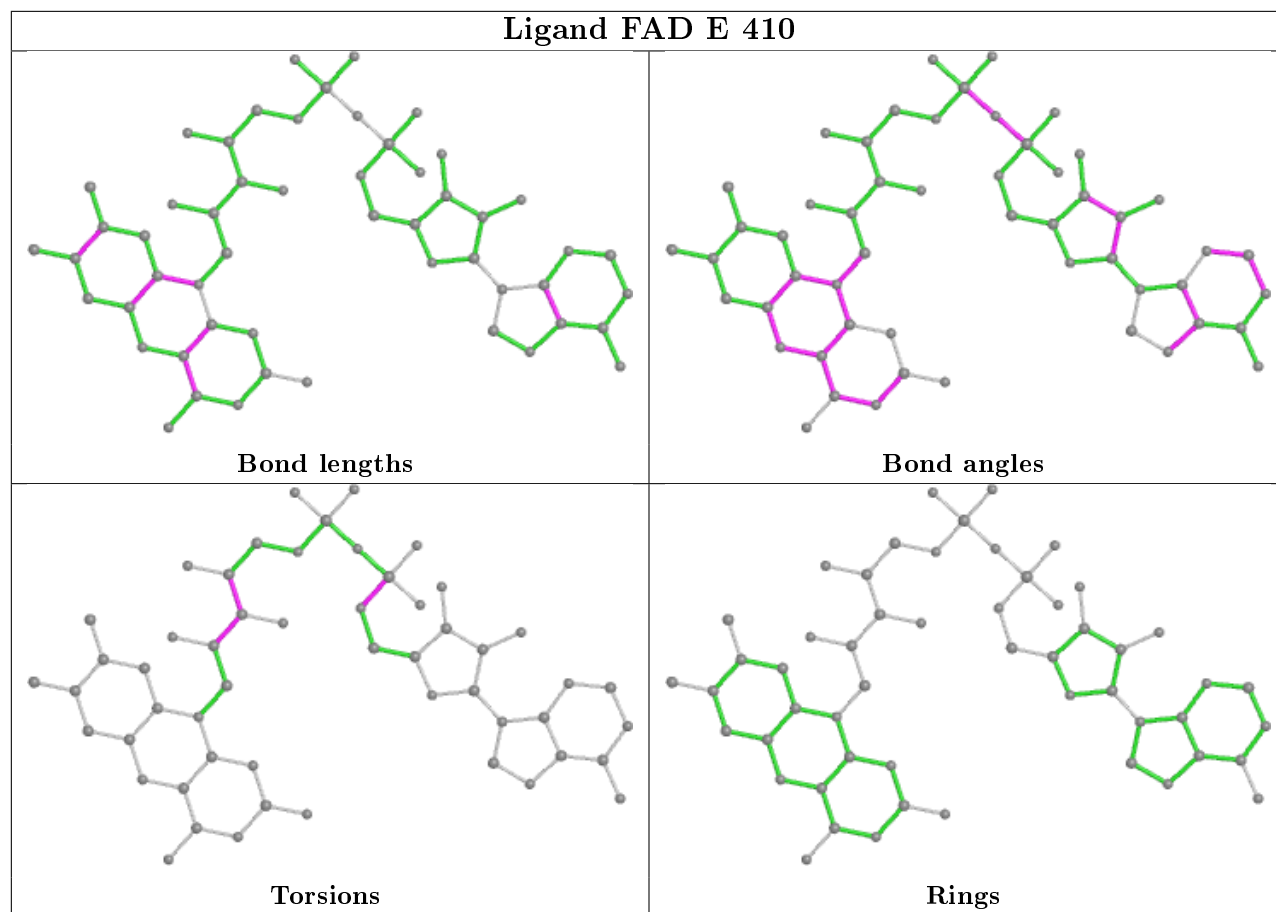




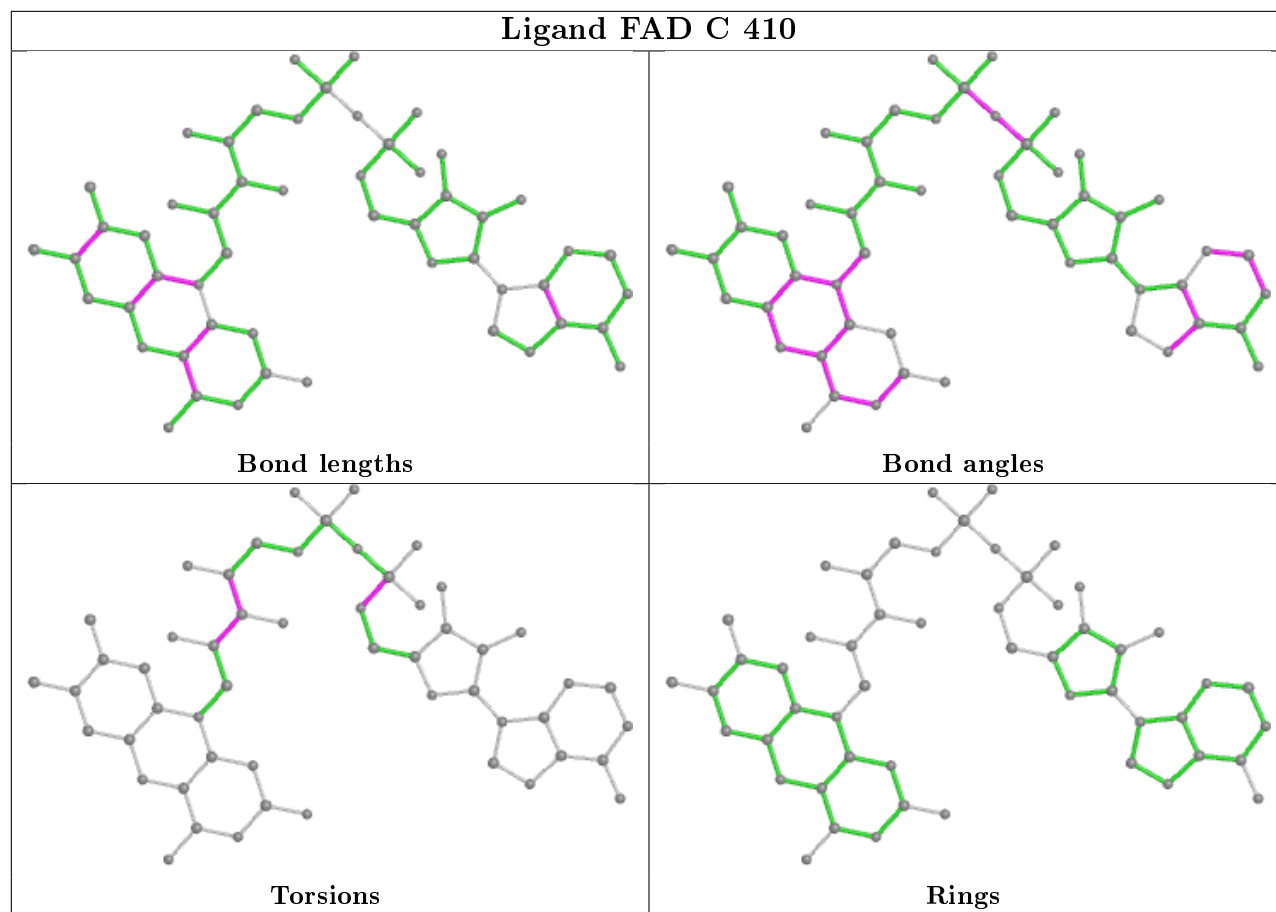


Ligand FAD B 410

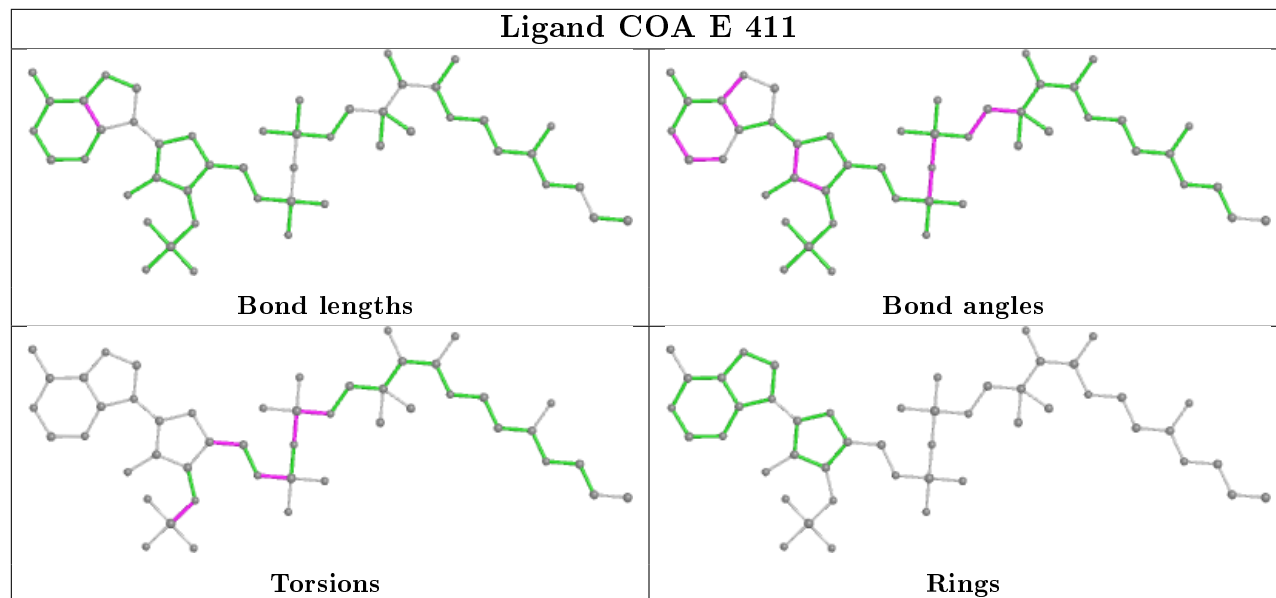


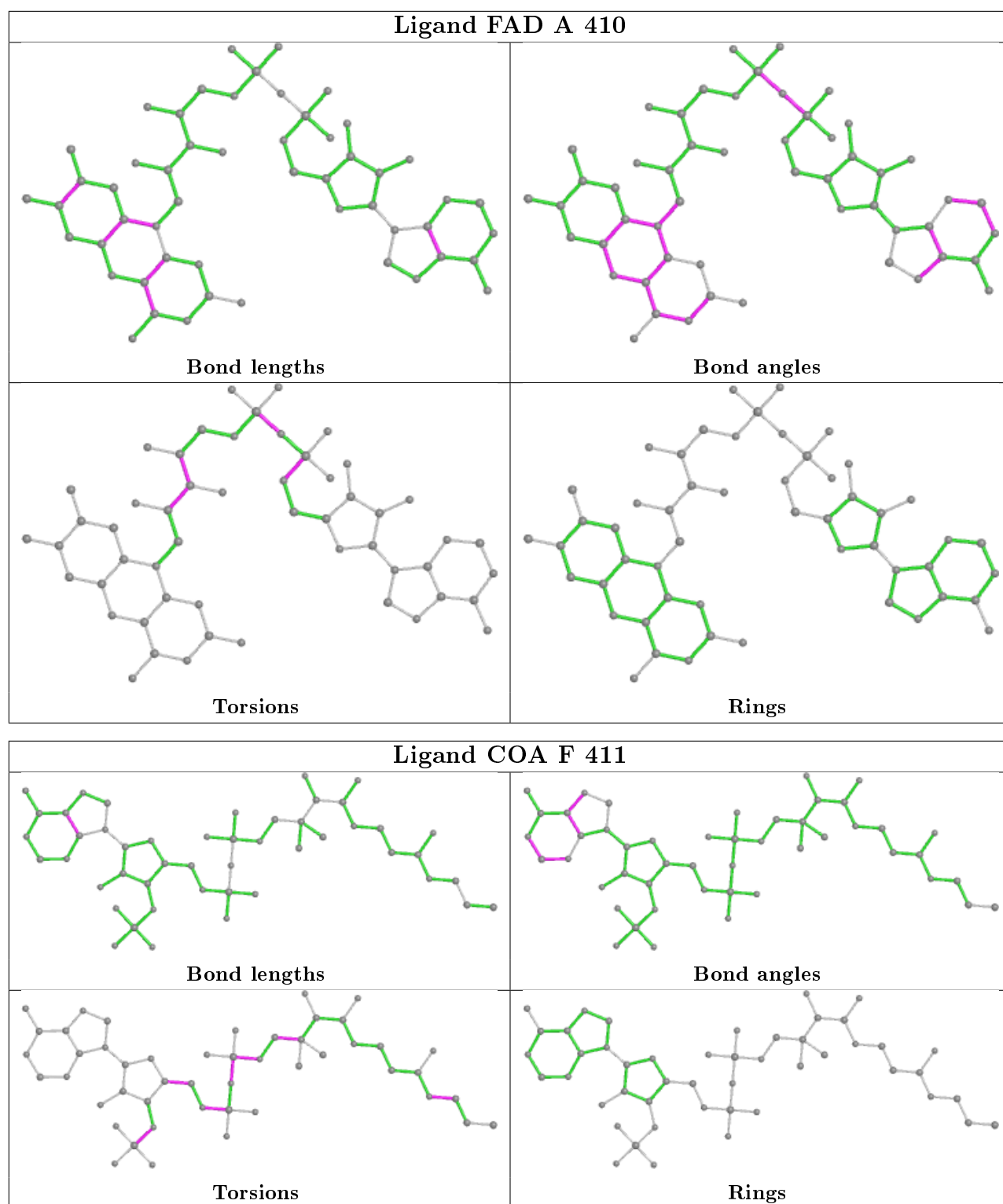


Ligand FAD C 410



Ligand COA E 411





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	391/401 (97%)	0.15	11 (2%)	53	60	29, 43, 68, 98	0
1	B	391/401 (97%)	0.27	15 (3%)	40	47	27, 45, 84, 112	0
1	C	391/401 (97%)	0.35	22 (5%)	24	30	31, 50, 81, 104	0
1	D	390/401 (97%)	0.16	18 (4%)	32	39	34, 53, 77, 106	0
1	E	391/401 (97%)	0.74	52 (13%)	3	4	30, 53, 89, 112	0
1	F	391/401 (97%)	0.92	72 (18%)	1	1	30, 58, 101, 119	0
All	All	2345/2406 (97%)	0.43	190 (8%)	12	16	27, 50, 89, 119	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	171	PHE	8.8
1	F	170	VAL	7.5
1	C	236	PHE	7.0
1	E	226	ILE	6.8
1	F	100	TYR	6.8
1	E	239	LEU	6.6
1	C	190	GLY	6.3
1	F	182	PHE	6.2
1	B	232	LEU	5.9
1	E	97	ILE	5.7
1	F	226	ILE	5.6
1	B	231	GLY	5.6
1	E	236	PHE	5.6
1	B	233	LYS	5.6
1	C	2	TYR	5.5
1	F	178	GLY	5.5
1	E	227	THR	5.3
1	C	233	LYS	5.3
1	F	150	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	228	PHE	5.2
1	F	215	PHE	5.1
1	E	178	GLY	5.0
1	C	147	ILE	4.8
1	E	224	MET	4.6
1	C	230	ASP	4.6
1	E	232	LEU	4.5
1	F	168	ALA	4.5
1	E	181	ALA	4.5
1	F	175	VAL	4.5
1	F	146	TYR	4.4
1	A	236	PHE	4.4
1	F	169	ARG	4.3
1	F	311	GLU	4.3
1	E	100	TYR	4.2
1	F	240	MET	4.1
1	C	231	GLY	4.1
1	F	220	ILE	4.1
1	F	313	PHE	4.1
1	F	192	GLU	4.0
1	C	243	TYR	4.0
1	E	228	PHE	3.9
1	F	109	ALA	3.9
1	F	217	ASP	3.9
1	F	111	ASP	3.9
1	A	190	GLY	3.8
1	C	148	LEU	3.8
1	D	167	PHE	3.8
1	A	234	ARG	3.8
1	B	230	ASP	3.7
1	F	179	ILE	3.7
1	F	190	GLY	3.7
1	C	173	ASP	3.7
1	F	139	ALA	3.6
1	F	227	THR	3.6
1	F	148	LEU	3.6
1	E	51	GLY	3.6
1	F	181	ALA	3.5
1	E	182	PHE	3.5
1	E	139	ALA	3.5
1	B	179	ILE	3.5
1	F	173	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	172	ASP	3.4
1	E	314	PRO	3.4
1	C	234	ARG	3.4
1	E	169	ARG	3.4
1	F	218	LEU	3.4
1	C	218	LEU	3.4
1	D	172	ASP	3.3
1	E	167	PHE	3.3
1	E	132	ALA	3.3
1	F	194	LEU	3.3
1	C	189	HIS	3.3
1	E	222	LYS	3.3
1	F	123	ILE	3.2
1	B	228	PHE	3.2
1	F	113	VAL	3.2
1	F	141	LYS	3.2
1	F	193	GLY	3.2
1	F	235	GLY	3.2
1	A	243	TYR	3.2
1	F	138	ARG	3.2
1	C	220	ILE	3.1
1	D	60	GLY	3.1
1	E	235	GLY	3.1
1	B	170	VAL	3.1
1	E	234	ARG	3.1
1	C	146	TYR	3.1
1	E	68	THR	3.0
1	F	243	TYR	3.0
1	E	171	PHE	3.0
1	E	133	SER	3.0
1	E	313	PHE	3.0
1	D	179	ILE	3.0
1	B	236	PHE	2.9
1	F	94	ILE	2.9
1	F	239	LEU	2.9
1	D	189	HIS	2.9
1	C	170	VAL	2.9
1	E	93	ALA	2.9
1	F	183	ILE	2.8
1	A	194	LEU	2.8
1	B	176	GLU	2.8
1	E	219	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	229	PRO	2.7
1	F	165	LEU	2.7
1	D	234	ARG	2.7
1	F	174	GLY	2.7
1	B	148	LEU	2.7
1	D	190	GLY	2.7
1	E	2	TYR	2.7
1	B	173	ASP	2.7
1	E	166	ILE	2.7
1	F	2	TYR	2.7
1	F	149	ASN	2.6
1	E	168	ALA	2.6
1	F	101	GLY	2.6
1	E	317	ASN	2.6
1	C	141	LYS	2.6
1	F	163	LEU	2.6
1	E	240	MET	2.6
1	E	312	THR	2.5
1	D	139	ALA	2.5
1	D	146	TYR	2.5
1	F	121	ILE	2.5
1	F	92	GLY	2.5
1	E	147	ILE	2.5
1	F	244	ASN	2.5
1	B	383	MET	2.4
1	E	243	TYR	2.4
1	F	229	PRO	2.4
1	E	165	LEU	2.4
1	F	242	ALA	2.4
1	F	241	SER	2.4
1	D	230	ASP	2.4
1	E	150	GLY	2.4
1	E	221	HIS	2.4
1	F	230	ASP	2.4
1	E	230	ASP	2.4
1	C	245	ALA	2.4
1	C	179	ILE	2.3
1	E	375	GLN	2.3
1	B	234	ARG	2.3
1	B	147	ILE	2.3
1	C	232	LEU	2.3
1	F	180	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	106	ILE	2.3
1	F	232	LEU	2.3
1	C	172	ASP	2.3
1	F	99	LYS	2.3
1	D	219	LYS	2.3
1	A	146	TYR	2.3
1	F	122	CYS	2.3
1	F	167	PHE	2.3
1	A	232	LEU	2.2
1	F	128	ALA	2.2
1	F	145	HIS	2.2
1	A	246[A]	GLN	2.2
1	D	148	LEU	2.2
1	F	53	MET	2.2
1	D	173	ASP	2.2
1	D	236	PHE	2.2
1	C	168	ALA	2.2
1	E	145	HIS	2.2
1	A	186	LEU	2.2
1	E	91	LEU	2.2
1	A	229	PRO	2.2
1	F	135	MET	2.2
1	E	106	ILE	2.1
1	F	129	GLY	2.1
1	D	235	GLY	2.1
1	D	171	PHE	2.1
1	E	140	ASP	2.1
1	D	243	TYR	2.1
1	F	222	LYS	2.1
1	E	248	VAL	2.1
1	E	215	PHE	2.1
1	F	375	GLN	2.0
1	A	239	LEU	2.0
1	E	123	ILE	2.0
1	F	216	HIS	2.0
1	F	234	ARG	2.0
1	E	225	MET	2.0
1	F	231	GLY	2.0
1	F	237	ALA	2.0
1	D	175	VAL	2.0
1	E	170	VAL	2.0
1	E	149	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	172	ASP	2.0
1	E	316	ILE	2.0
1	F	312	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

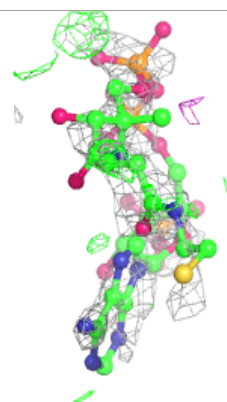
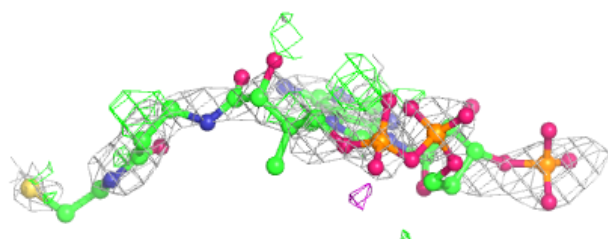
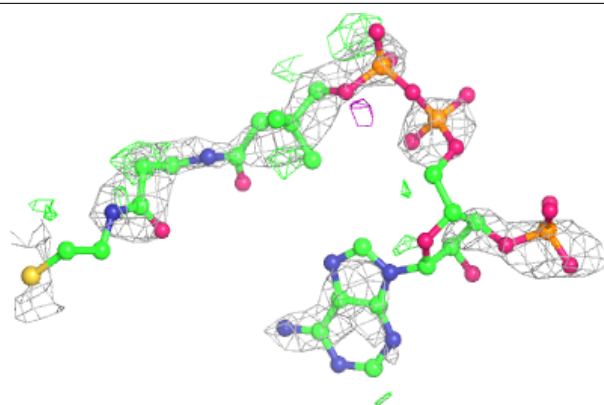
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	COA	A	411	48/48	0.67	0.47	41,56,69,76	48
3	COA	E	411	48/48	0.75	0.40	58,66,75,91	48
3	COA	D	411	48/48	0.76	0.34	43,60,75,77	48
5	SO4	C	1393	5/5	0.79	0.28	83,88,102,163	0
3	COA	B	411	48/48	0.80	0.33	48,60,72,77	48
3	COA	F	411	48/48	0.83	0.26	61,71,79,115	48
4	SIN	C	412	8/8	0.91	0.36	39,60,75,98	0
2	FAD	E	410	53/53	0.94	0.16	35,53,64,68	0
2	FAD	F	410	53/53	0.95	0.14	50,61,77,84	0
2	FAD	B	410	53/53	0.96	0.14	29,42,52,57	0
2	FAD	A	410	53/53	0.97	0.16	26,33,47,51	0
2	FAD	C	410	53/53	0.97	0.15	28,39,52,64	0
2	FAD	D	410	53/53	0.97	0.15	31,40,54,62	0

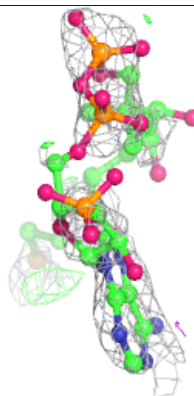
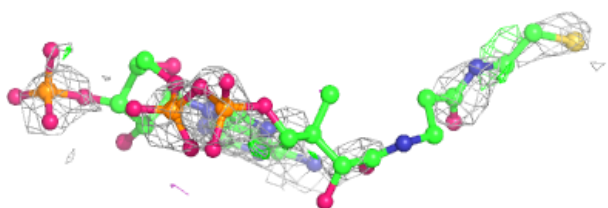
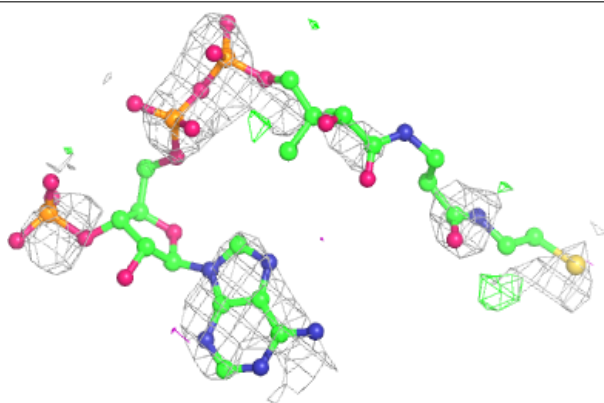
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around COA A 411:

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

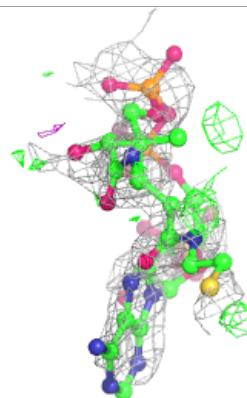
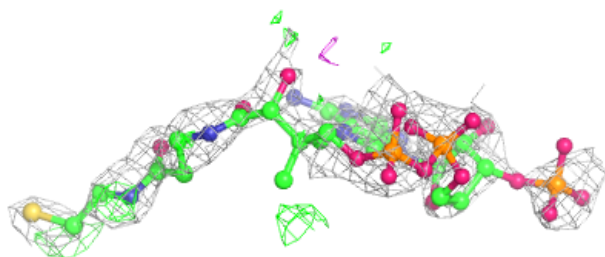
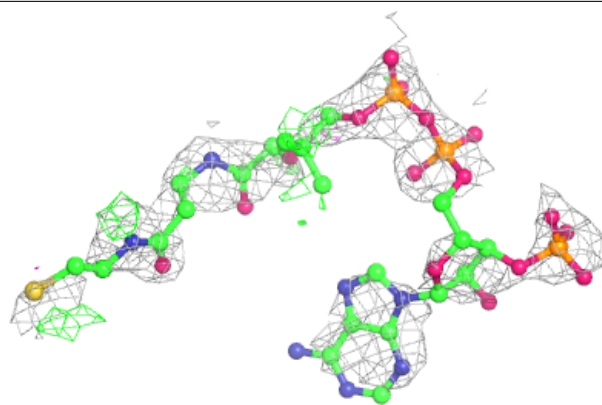
**Electron density around COA E 411:**

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

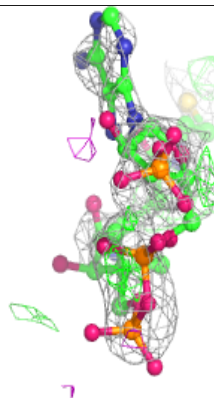
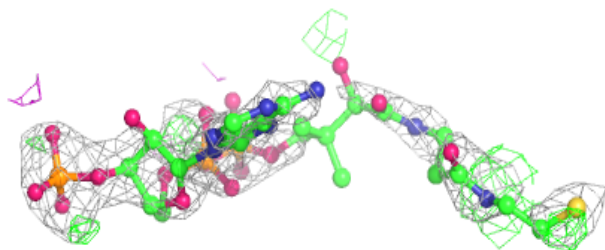
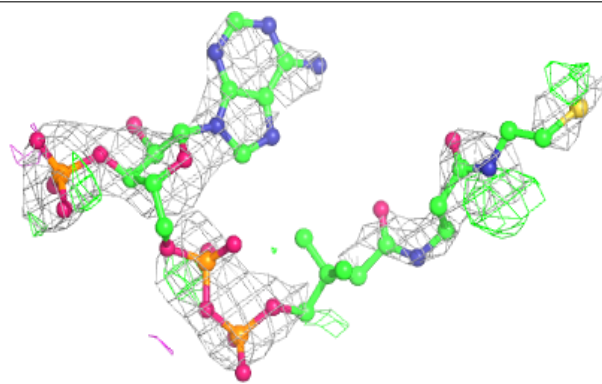


Electron density around COA D 411:

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

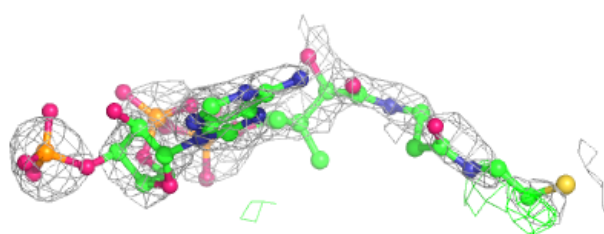
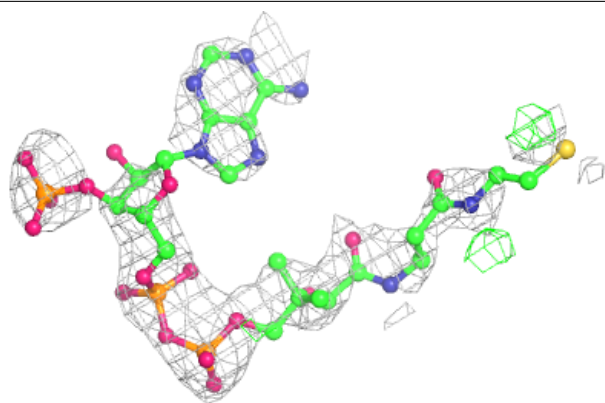
**Electron density around COA B 411:**

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

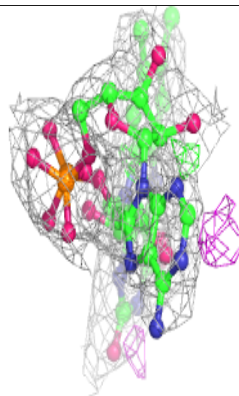
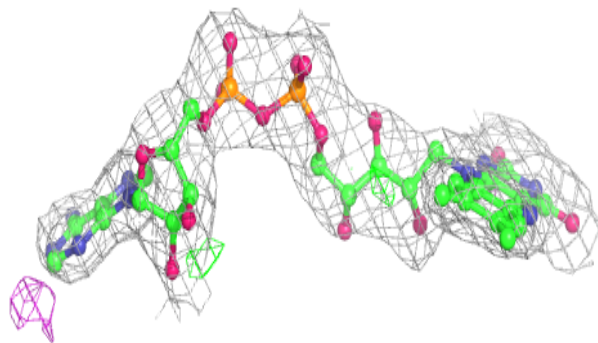
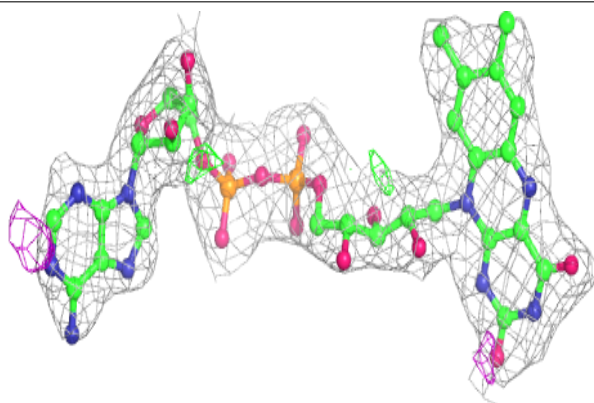


Electron density around COA F 411:

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

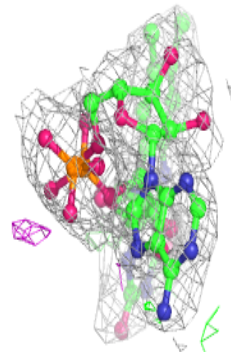
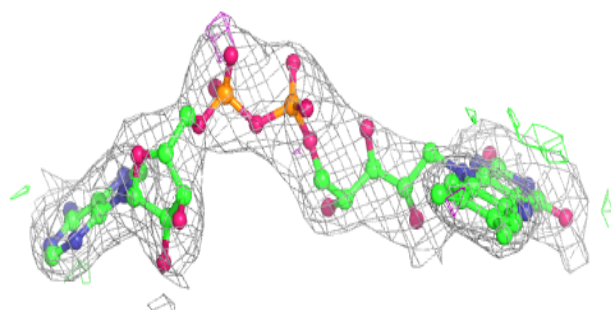
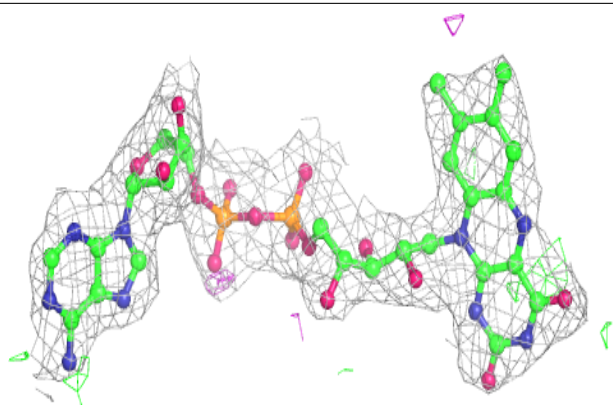
**Electron density around FAD E 410:**

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

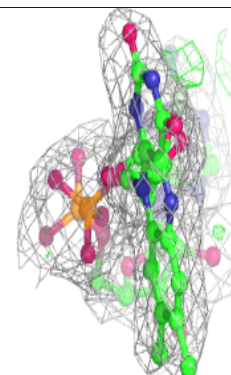
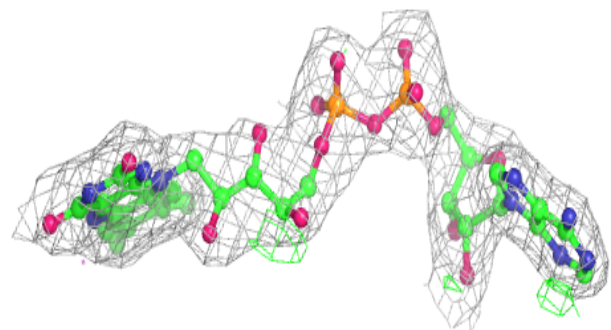
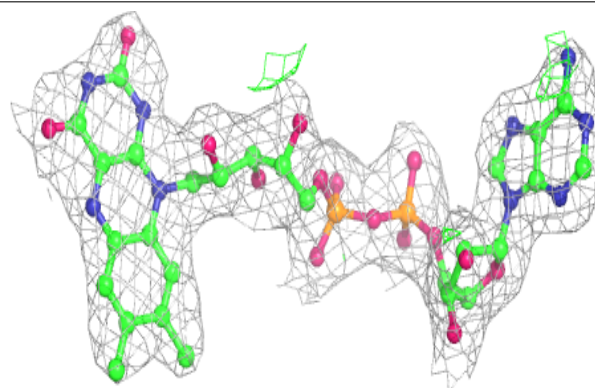


Electron density around FAD F 410:

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

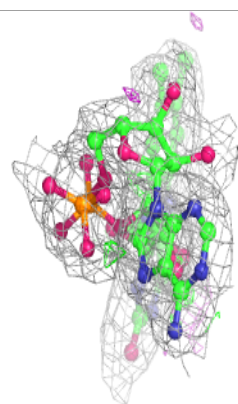
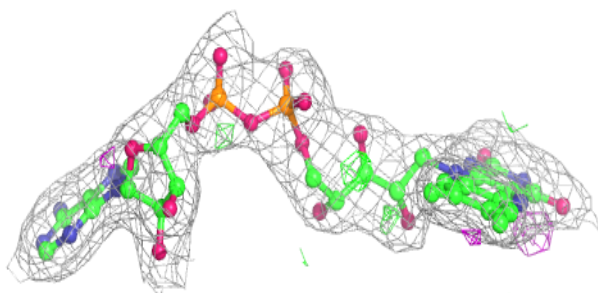
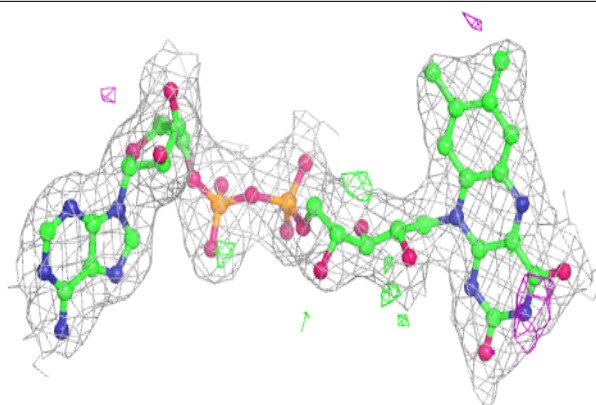
**Electron density around FAD B 410:**

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

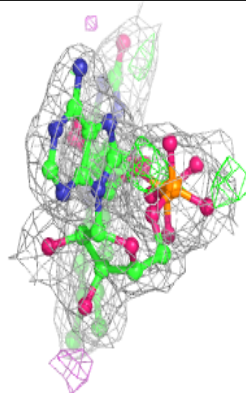
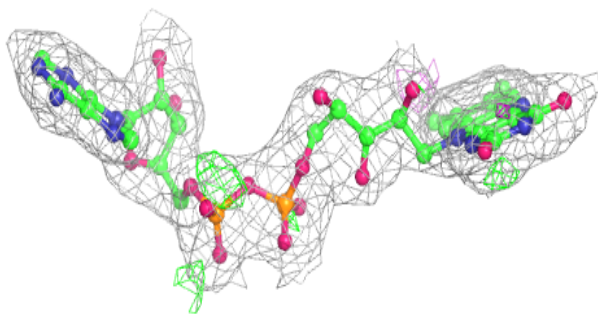
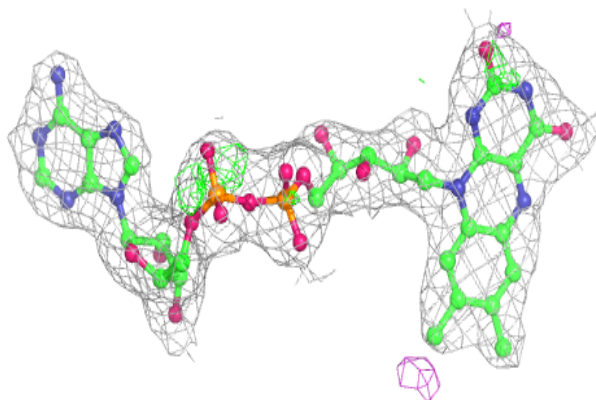


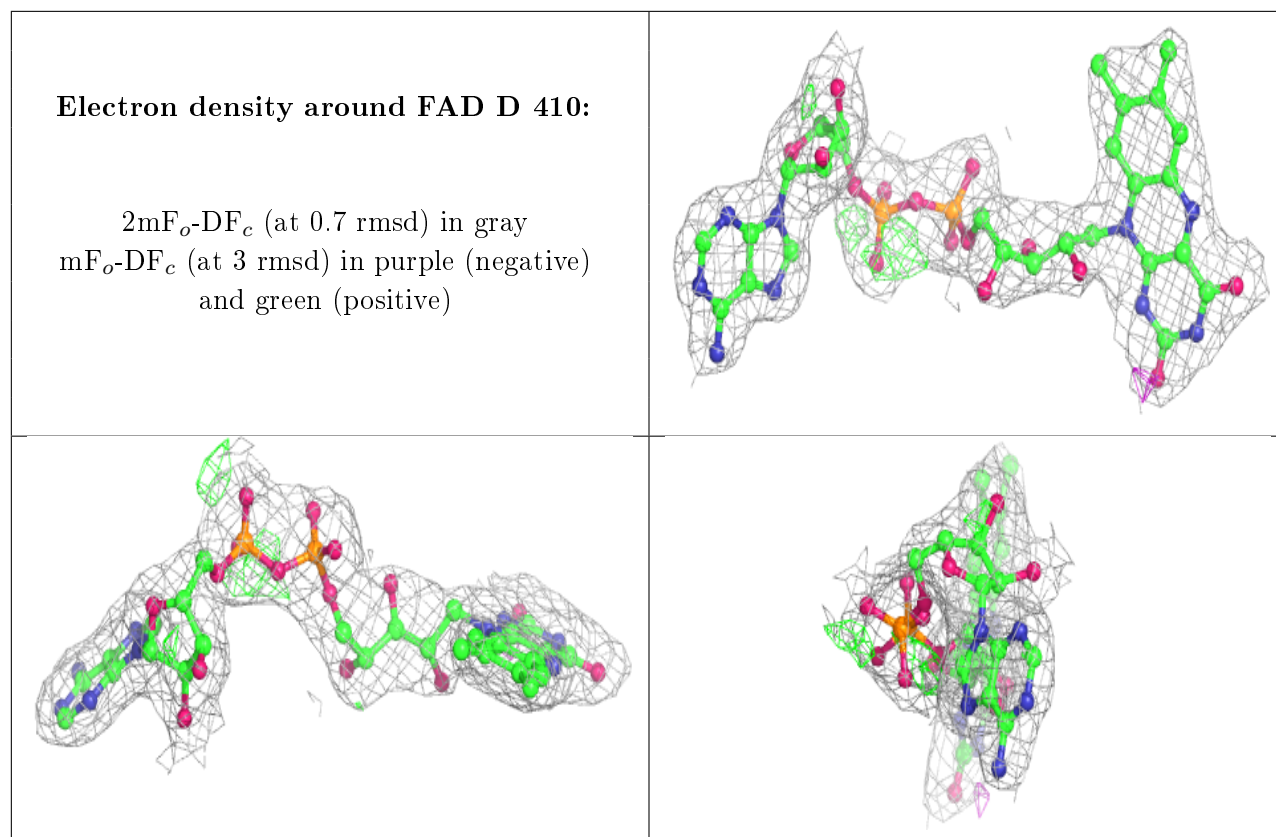
Electron density around FAD A 410:

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

**Electron density around FAD C 410:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.