



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:10 AM UTC

PDB ID : 5AHS / pdb_00005ahs
Title : 3-Sulfinopropionyl-Coenzyme A (3SP-CoA) desulfonase from *Advenella minghamensis* 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

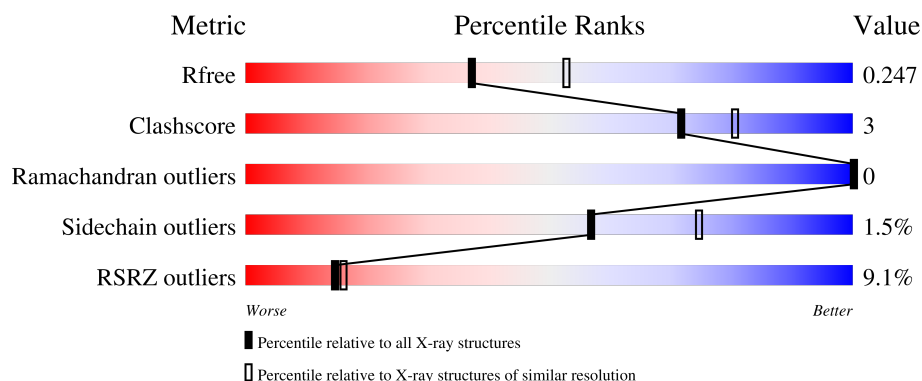
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

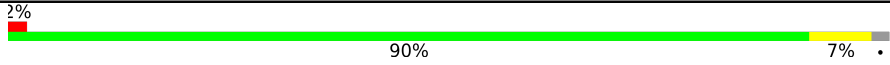
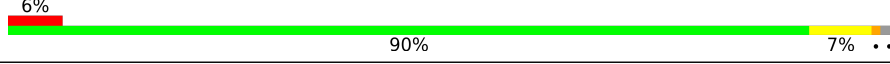
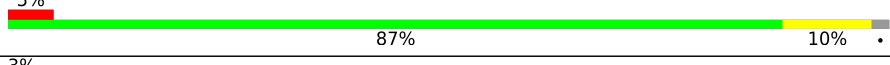
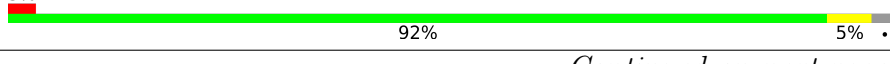
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	401	
1	C	401	
1	D	401	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	401	16% 88% 9%
1	F	401	21% 88% 9%

2 Entry composition [i](#)

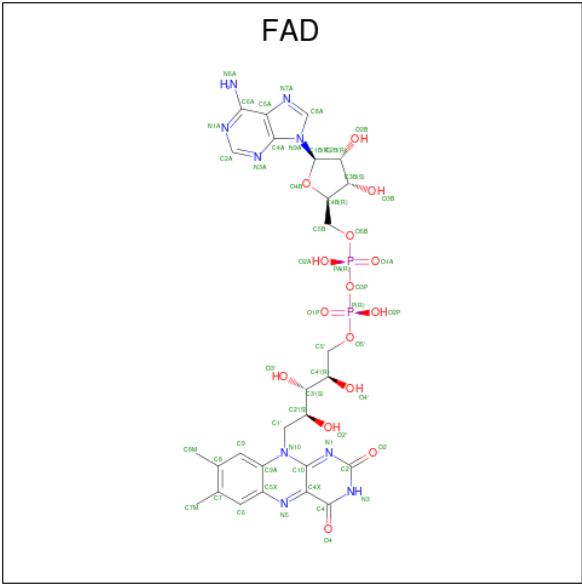
There are 6 unique types of molecules in this entry. The entry contains 19886 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

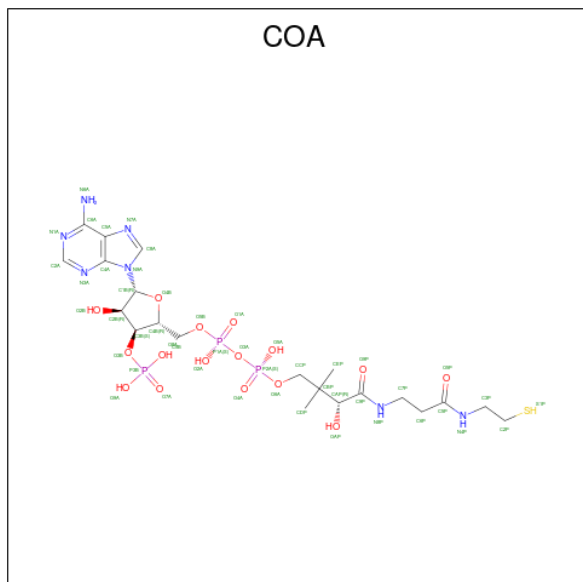
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	1	0
			2980	1871	527	563	19			
1	B	391	Total	C	N	O	S	0	1	0
			2983	1872	528	564	19			
1	C	391	Total	C	N	O	S	0	0	0
			2974	1867	526	562	19			
1	D	390	Total	C	N	O	S	0	0	0
			2962	1858	525	560	19			
1	E	391	Total	C	N	O	S	0	0	0
			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 (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



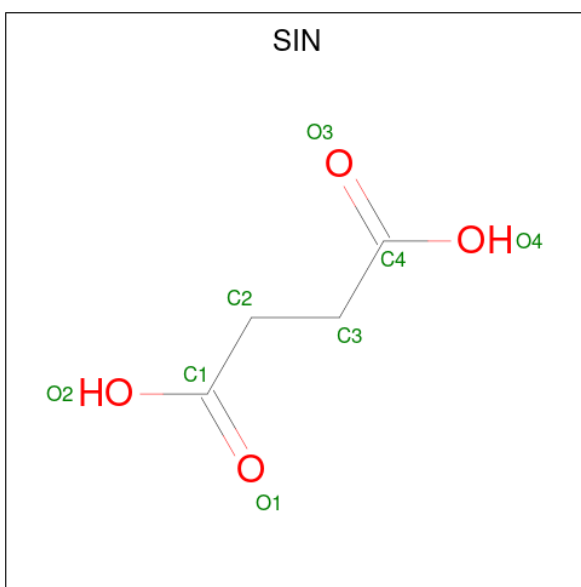
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



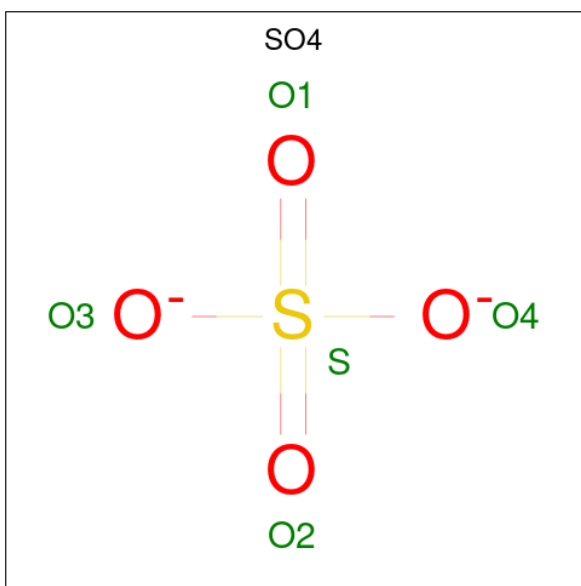
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	E	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	F	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 4 is SUCCINIC ACID (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



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

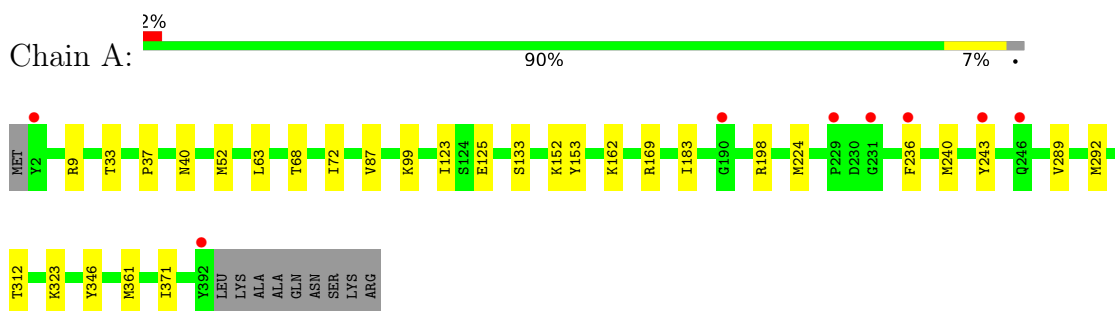
- Molecule 6 is water.

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

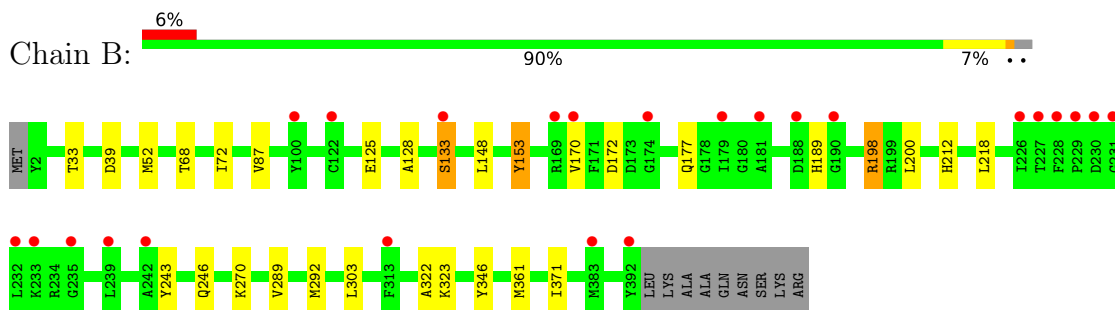
3 Residue-property plots [i](#)

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

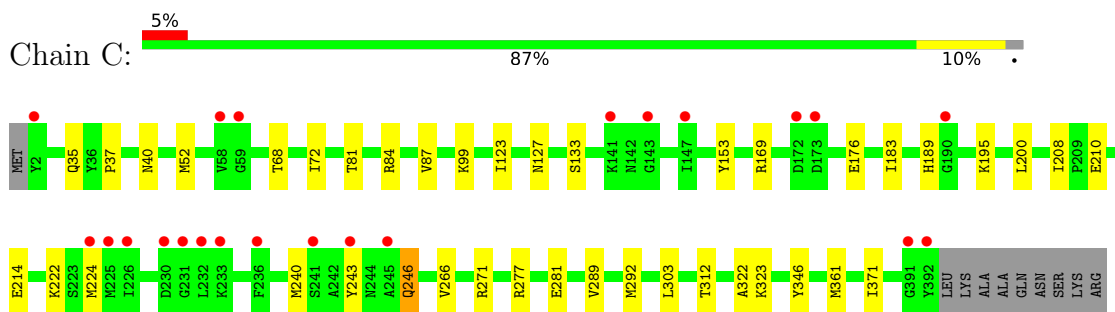
• Molecule 1: ACYL-COA DEHYDROGENASE



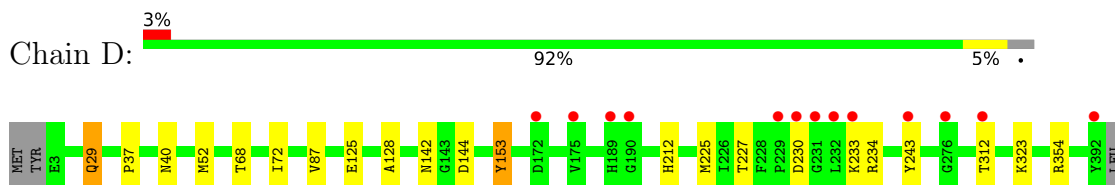
• Molecule 1: ACYL-COA DEHYDROGENASE



• Molecule 1: ACYL-COA DEHYDROGENASE



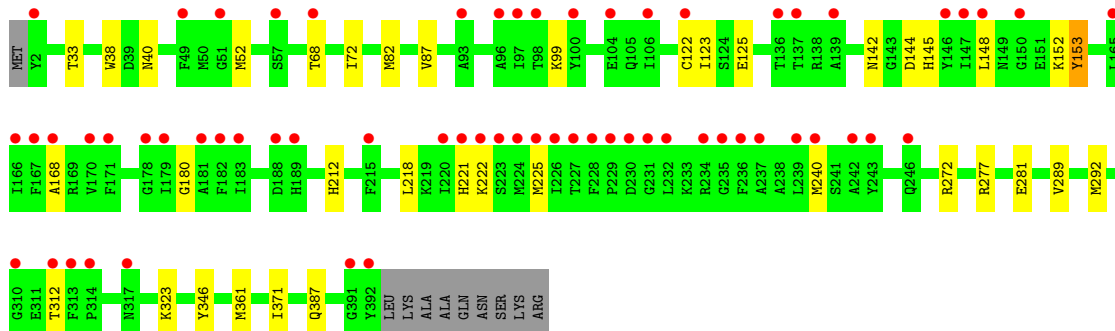
• Molecule 1: ACYL-COA DEHYDROGENASE



LYS
ALA
ALA
GLN
ASN
SER
LYS
ARG

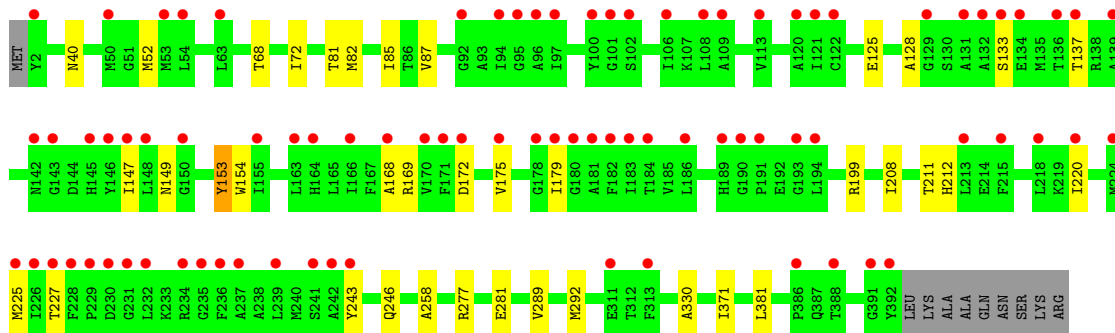
● Molecule 1: ACYL-COA DEHYDROGENASE

Chain E: 16% 88% 9%



● Molecule 1: ACYL-COA DEHYDROGENASE

Chain F: 21% 88% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.07Å 233.49Å 121.28Å 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 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.200 , 0.244 0.207 , 0.247	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)	0.35 , 49.9	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.27	0/3034	0.66	0/4095
1	B	0.27	0/3034	0.66	0/4095
1	C	0.27	0/3025	0.67	0/4083
1	D	0.26	0/3012	0.67	0/4065
1	E	0.27	0/3025	0.68	0/4083
1	F	0.27	0/3034	0.68	0/4095
All	All	0.27	0/18164	0.67	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 [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	2980	0	2971	20	0
1	B	2983	0	2970	19	0
1	C	2974	0	2963	24	0
1	D	2962	0	2954	14	0
1	E	2974	0	2963	25	0
1	F	2980	0	2971	18	0
2	A	53	0	31	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	0	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	2	0
All	All	19886	0	18142	119	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 (119) 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:123:ILE:HD13	1:C:240:MET:HE1	1.79	0.65
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:E:289:VAL:HA	1:E:292:MET:HE2	1.83	0.61
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:123:ILE:HD13	1:E:240:MET:HE1	1.87	0.57
1:C:133:SER:O	1:C:169:ARG:NH2	2.38	0.56
1:A:123:ILE:HD13	1:A:240:MET:HE1	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:D:52:MET:HE3	1:D:68:THR:HG22	1.89	0.55
1:B:289:VAL:HA	1:B:292:MET:HE2	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:C:52:MET:HE3	1:C:68:THR:HG22	1.92	0.52
1:B:72:ILE:HD13	1:B:87:VAL:HG22	1.91	0.52
1:A:52:MET:HE3	1:A:68:THR:HG22	1.91	0.52
1:A:346:TYR:CZ	1:B:361:MET:HB3	2.45	0.52
1:F:52:MET:HE3	1:F:68:THR:HG22	1.92	0.52
1:B:125:GLU:HB2	1:B:128:ALA:HB3	1.92	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:B:52:MET:HE3	1:B:68:THR:HG22	1.93	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:A:289:VAL:HA	1:A:292:MET:HE2	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:E:52:MET:HE3	1:E:68:THR:HG22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:410:FAD:HO2'	3:D:411:COA:HS1	1.51	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:B:323:LYS:NZ	6:B:2226:HOH:O	2.47	0.46
1:F:225:MET:HE3	1:F:227:THR:HG22	1.97	0.46
1:D:37:PRO:HB2	1:D:40:ASN:HB2	1.97	0.46
1:A:183:ILE:HB	1:A:224:MET:HE3	1.97	0.46
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:D:142:ASN:ND2	6:D:2110:HOH:O	2.49	0.45
1:D:225:MET:HE3	1:D:227:THR:HG22	1.97	0.45
1:C:289:VAL:HA	1:C:292:MET:HE2	1.99	0.45
1:C:323:LYS:NZ	6:C:2150:HOH:O	2.48	0.45
1:B:198:ARG:NH1	6:B:2157:HOH:O	2.49	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:40:ASN:HB3	1:E:82:MET:SD	2.57	0.44
1:E:323:LYS:NZ	6:E:2163:HOH:O	2.51	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:C:183:ILE:HB	1:C:224:MET:HE3	2.00	0.43
1:E:148:LEU:HB2	1:E:218:LEU:HB3	2.01	0.43
1:F:289:VAL:HA	1:F:292:MET:HE2	2.00	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:F:82:MET:HE2	1:F:85:ILE:HD12	1.99	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:195:LYS:HB3	1:C:214:GLU:HB2	2.02	0.42
1:C:99:LYS:HD3	1:C:312:THR:HG21	2.02	0.41
1:D:29:GLN:HE21	1:D:29:GLN:HA	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
1:F:154:TRP:NE1	6:F:2091:HOH:O	2.43	0.41
1:A:72:ILE:HD13	1:A:87:VAL:HG22	2.01	0.41
1:A:99:LYS:HD3	1:A:312:THR:HG21	2.03	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:OD1	1:B:39:ASP:N	2.55	0.40
1:C:266:VAL:HG13	1:F:381:LEU:HD23	2.03	0.40
1:D:233:LYS:NZ	6:D:2122:HOH:O	2.52	0.40

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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	76	87
1	B	304/311 (98%)	298 (98%)	6 (2%)	48	67
1	C	303/311 (97%)	297 (98%)	6 (2%)	48	67
1	D	302/311 (97%)	299 (99%)	3 (1%)	68	82
1	E	303/311 (97%)	300 (99%)	3 (1%)	68	82
1	F	304/311 (98%)	296 (97%)	8 (3%)	40	59
All	All	1820/1866 (98%)	1792 (98%)	28 (2%)	57	75

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	TYR
1	A	371	ILE
1	B	133	SER
1	B	153	TYR
1	B	172	ASP
1	B	189	HIS
1	B	198	ARG
1	B	371	ILE
1	C	153	TYR
1	C	189	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	222	LYS
1	C	243	TYR
1	C	246	GLN
1	C	371	ILE
1	D	29	GLN
1	D	153	TYR
1	D	312	THR
1	E	153	TYR
1	E	225	MET
1	E	371	ILE
1	F	147	ILE
1	F	149	ASN
1	F	153	TYR
1	F	179	ILE
1	F	220	ILE
1	F	246[A]	GLN
1	F	246[B]	GLN
1	F	371	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	375	GLN
1	B	35	GLN
1	B	127	ASN
1	B	212	HIS
1	B	283	GLN
1	C	375	GLN
1	D	29	GLN
1	D	212	HIS
1	D	355	HIS
1	D	370	GLN
1	E	127	ASN
1	E	212	HIS
1	E	246	GLN
1	E	295	GLN
1	F	212	HIS
1	F	295	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
2	FAD	C	410	-	58,58,58	1.43	9 (15%)	85,89,89	1.54	15 (17%)
2	FAD	E	410	-	58,58,58	1.46	9 (15%)	85,89,89	1.54	14 (16%)
4	SIN	C	412	-	7,7,7	1.02	0	8,8,8	1.42	0
3	COA	F	411	-	47,50,50	1.21	6 (12%)	69,75,75	1.49	9 (13%)
2	FAD	F	410	-	58,58,58	1.45	8 (13%)	85,89,89	1.56	16 (18%)
2	FAD	A	410	-	58,58,58	1.45	9 (15%)	85,89,89	1.54	15 (17%)
2	FAD	D	410	-	58,58,58	1.45	10 (17%)	85,89,89	1.53	16 (18%)
3	COA	E	411	-	47,50,50	1.16	4 (8%)	69,75,75	1.55	11 (15%)
2	FAD	B	410	-	58,58,58	1.47	9 (15%)	85,89,89	1.53	15 (17%)
3	COA	A	411	-	47,50,50	1.18	4 (8%)	69,75,75	1.49	9 (13%)
3	COA	D	411	-	47,50,50	1.18	4 (8%)	69,75,75	1.50	10 (14%)
5	SO4	C	1393	-	4,4,4	0.41	0	6,6,6	0.66	0
3	COA	B	411	-	47,50,50	1.16	4 (8%)	69,75,75	1.50	9 (13%)

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
2	FAD	C	410	-	-	11/34/50/50	0/6/6/6
2	FAD	E	410	-	-	9/34/50/50	0/6/6/6
4	SIN	C	412	-	-	0/5/5/5	-
3	COA	F	411	-	-	14/48/64/64	0/3/3/3
2	FAD	F	410	-	-	7/34/50/50	0/6/6/6
2	FAD	A	410	-	-	10/34/50/50	0/6/6/6
2	FAD	D	410	-	-	10/34/50/50	0/6/6/6
3	COA	E	411	-	-	12/48/64/64	0/3/3/3
2	FAD	B	410	-	-	8/34/50/50	0/6/6/6
3	COA	A	411	-	-	9/48/64/64	0/3/3/3
3	COA	D	411	-	-	5/48/64/64	0/3/3/3
3	COA	B	411	-	-	11/48/64/64	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	410	FAD	C9A-C5X	5.28	1.49	1.41
2	E	410	FAD	C9A-C5X	5.28	1.49	1.41
2	F	410	FAD	C9A-C5X	5.28	1.49	1.41
2	B	410	FAD	C9A-C5X	5.25	1.49	1.41
2	D	410	FAD	C9A-C5X	5.24	1.49	1.41
2	C	410	FAD	C9A-C5X	5.22	1.49	1.41
3	A	411	COA	C5A-C4A	4.71	1.47	1.39
3	E	411	COA	C5A-C4A	4.71	1.47	1.39
2	D	410	FAD	C5A-C4A	4.70	1.47	1.39
3	B	411	COA	C5A-C4A	4.68	1.47	1.39
2	B	410	FAD	C5A-C4A	4.67	1.47	1.39
2	F	410	FAD	C5A-C4A	4.67	1.47	1.39
3	F	411	COA	C5A-C4A	4.66	1.47	1.39
2	E	410	FAD	C5A-C4A	4.66	1.47	1.39
3	D	411	COA	C5A-C4A	4.66	1.47	1.39
2	A	410	FAD	C5A-C4A	4.65	1.47	1.39
2	C	410	FAD	C5A-C4A	4.59	1.47	1.39
2	F	410	FAD	C8-C7	3.39	1.49	1.40
2	E	410	FAD	C8-C7	3.36	1.49	1.40
2	A	410	FAD	C8-C7	3.36	1.49	1.40
2	B	410	FAD	C8-C7	3.35	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	410	FAD	C8-C7	3.32	1.49	1.40
2	C	410	FAD	C8-C7	3.32	1.48	1.40
3	E	411	COA	C5A-C6A	2.76	1.48	1.41
3	F	411	COA	C5A-C6A	2.75	1.48	1.41
3	D	411	COA	C5A-C6A	2.75	1.48	1.41
3	B	411	COA	C5A-C6A	2.74	1.48	1.41
2	D	410	FAD	C5A-C6A	2.72	1.48	1.41
2	B	410	FAD	C5A-C6A	2.72	1.48	1.41
3	A	411	COA	C5A-C6A	2.71	1.48	1.41
2	F	410	FAD	C5A-C6A	2.69	1.48	1.41
2	E	410	FAD	C5A-C6A	2.69	1.48	1.41
2	A	410	FAD	C5A-C6A	2.67	1.48	1.41
2	C	410	FAD	C5A-C6A	2.62	1.48	1.41
3	F	411	COA	P2A-O3A	2.58	1.62	1.59
2	B	410	FAD	C4-N3	-2.54	1.34	1.38
2	E	410	FAD	C4-N3	-2.48	1.34	1.38
2	F	410	FAD	C4-N3	-2.47	1.34	1.38
3	B	411	COA	C8A-N7A	2.42	1.36	1.31
3	D	411	COA	C8A-N7A	2.41	1.36	1.31
3	A	411	COA	C8A-N7A	2.40	1.36	1.31
2	D	410	FAD	C8A-N7A	2.40	1.36	1.31
2	A	410	FAD	C4-N3	-2.39	1.34	1.38
3	E	411	COA	C8A-N7A	2.39	1.36	1.31
2	D	410	FAD	C4-N3	-2.39	1.34	1.38
2	C	410	FAD	C4-N3	-2.38	1.34	1.38
3	F	411	COA	P1A-O3A	2.38	1.62	1.59
2	A	410	FAD	C8A-N7A	2.37	1.36	1.31
3	F	411	COA	C8A-N7A	2.37	1.36	1.31
2	B	410	FAD	C8A-N7A	2.37	1.36	1.31
2	F	410	FAD	C8A-N7A	2.36	1.36	1.31
2	E	410	FAD	C8A-N7A	2.34	1.36	1.31
2	C	410	FAD	C5A-N7A	-2.33	1.34	1.39
3	D	411	COA	C5A-N7A	-2.28	1.34	1.39
2	C	410	FAD	C8A-N7A	2.27	1.36	1.31
2	B	410	FAD	C5A-N7A	-2.26	1.35	1.39
2	F	410	FAD	C5A-N7A	-2.26	1.35	1.39
2	F	410	FAD	C4X-N5	2.26	1.35	1.30
2	E	410	FAD	C5A-N7A	-2.25	1.35	1.39
3	B	411	COA	C5A-N7A	-2.23	1.35	1.39
3	A	411	COA	C5A-N7A	-2.21	1.35	1.39
3	E	411	COA	C5A-N7A	-2.21	1.35	1.39
2	E	410	FAD	C4X-N5	2.19	1.35	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	410	FAD	C4X-N5	2.19	1.35	1.30
2	C	410	FAD	C4X-N5	2.19	1.35	1.30
2	D	410	FAD	C5A-N7A	-2.18	1.35	1.39
3	F	411	COA	C5A-N7A	-2.18	1.35	1.39
2	A	410	FAD	C5A-N7A	-2.16	1.35	1.39
2	D	410	FAD	C4X-N5	2.15	1.35	1.30
2	A	410	FAD	C4X-N5	2.13	1.35	1.30
2	D	410	FAD	C5X-N5	-2.08	1.35	1.39
2	A	410	FAD	C5X-N5	-2.07	1.35	1.39
2	E	410	FAD	C5X-N5	-2.04	1.35	1.39
2	B	410	FAD	C5X-N5	-2.02	1.35	1.39
2	D	410	FAD	C4A-N9A	-2.02	1.33	1.37
2	C	410	FAD	C5X-N5	-2.00	1.35	1.39

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	411	COA	C5A-C4A-N3A	-5.84	118.68	126.72
3	F	411	COA	C5A-C4A-N3A	-5.77	118.78	126.72
3	B	411	COA	C5A-C4A-N3A	-5.76	118.79	126.72
2	E	410	FAD	C5A-C4A-N3A	-5.75	118.81	126.72
2	F	410	FAD	C5A-C4A-N3A	-5.72	118.84	126.72
3	A	411	COA	C5A-C4A-N3A	-5.71	118.86	126.72
3	D	411	COA	C5A-C4A-N3A	-5.70	118.87	126.72
2	B	410	FAD	C5A-C4A-N3A	-5.65	118.94	126.72
2	A	410	FAD	C5A-C4A-N3A	-5.62	118.98	126.72
2	C	410	FAD	C5A-C4A-N3A	-5.59	119.01	126.72
2	D	410	FAD	C5A-C4A-N3A	-5.52	119.12	126.72
3	E	411	COA	N3A-C4A-N9A	4.60	135.00	127.17
2	E	410	FAD	N3A-C4A-N9A	4.58	134.96	127.17
3	D	411	COA	N3A-C4A-N9A	4.56	134.93	127.17
3	B	411	COA	N3A-C4A-N9A	4.56	134.92	127.17
2	F	410	FAD	N3A-C4A-N9A	4.55	134.91	127.17
3	A	411	COA	N3A-C4A-N9A	4.55	134.90	127.17
3	F	411	COA	N3A-C4A-N9A	4.51	134.83	127.17
2	C	410	FAD	N3A-C4A-N9A	4.50	134.82	127.17
2	A	410	FAD	N3A-C4A-N9A	4.47	134.76	127.17
2	B	410	FAD	N3A-C4A-N9A	4.45	134.74	127.17
2	D	410	FAD	N3A-C4A-N9A	4.35	134.57	127.17
3	E	411	COA	C2A-N3A-C4A	3.74	120.95	111.83
3	F	411	COA	C2A-N3A-C4A	3.73	120.94	111.83
3	B	411	COA	C2A-N3A-C4A	3.72	120.91	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	410	FAD	C2A-N3A-C4A	3.69	120.84	111.83
3	A	411	COA	C2A-N3A-C4A	3.69	120.83	111.83
2	F	410	FAD	C2A-N3A-C4A	3.68	120.81	111.83
3	D	411	COA	C2A-N3A-C4A	3.66	120.76	111.83
2	B	410	FAD	C2A-N3A-C4A	3.65	120.75	111.83
2	A	410	FAD	C2A-N3A-C4A	3.60	120.63	111.83
2	D	410	FAD	C2A-N3A-C4A	3.60	120.62	111.83
2	C	410	FAD	C2A-N3A-C4A	3.59	120.61	111.83
3	E	411	COA	C4A-C5A-N7A	-3.53	106.55	110.58
3	F	411	COA	C4A-C5A-N7A	-3.52	106.56	110.58
2	A	410	FAD	C4A-C5A-N7A	-3.49	106.59	110.58
3	B	411	COA	C4A-C5A-N7A	-3.49	106.59	110.58
2	B	410	FAD	C4A-C5A-N7A	-3.48	106.60	110.58
2	D	410	FAD	C4A-C5A-N7A	-3.44	106.65	110.58
3	A	411	COA	C4A-C5A-N7A	-3.44	106.65	110.58
2	F	410	FAD	C4A-C5A-N7A	-3.42	106.67	110.58
2	C	410	FAD	C4A-C5A-N7A	-3.39	106.70	110.58
2	E	410	FAD	C4A-C5A-N7A	-3.39	106.70	110.58
3	D	411	COA	C4A-C5A-N7A	-3.36	106.74	110.58
3	F	411	COA	N3A-C2A-N1A	-3.29	123.61	128.58
3	B	411	COA	N3A-C2A-N1A	-3.28	123.61	128.58
2	B	410	FAD	N3A-C2A-N1A	-3.26	123.64	128.58
2	C	410	FAD	N3A-C2A-N1A	-3.26	123.64	128.58
3	A	411	COA	N3A-C2A-N1A	-3.26	123.65	128.58
2	F	410	FAD	N3A-C2A-N1A	-3.26	123.65	128.58
2	E	410	FAD	N3A-C2A-N1A	-3.25	123.66	128.58
3	D	411	COA	N3A-C2A-N1A	-3.25	123.67	128.58
3	E	411	COA	N3A-C2A-N1A	-3.23	123.69	128.58
2	D	410	FAD	N3A-C2A-N1A	-3.23	123.70	128.58
2	A	410	FAD	N3A-C2A-N1A	-3.21	123.73	128.58
2	F	410	FAD	C4-C4X-N5	3.06	122.44	118.21
2	C	410	FAD	C4A-N9A-C8A	2.88	108.77	105.74
2	A	410	FAD	C4A-N9A-C8A	2.88	108.77	105.74
2	C	410	FAD	C4-C4X-N5	2.80	122.08	118.21
2	D	410	FAD	C4A-N9A-C8A	2.79	108.67	105.74
3	D	411	COA	C4A-N9A-C8A	2.78	108.66	105.74
3	A	411	COA	C4A-N9A-C8A	2.76	108.63	105.74
2	E	410	FAD	C4-C4X-N5	2.74	121.99	118.21
2	F	410	FAD	C4A-N9A-C8A	2.73	108.61	105.74
3	B	411	COA	C4A-N9A-C8A	2.71	108.59	105.74
2	B	410	FAD	C4-C4X-N5	2.71	121.95	118.21
2	E	410	FAD	C4A-N9A-C8A	2.68	108.55	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	411	COA	C4A-N9A-C8A	2.67	108.55	105.74
2	B	410	FAD	C4A-N9A-C8A	2.67	108.54	105.74
3	F	411	COA	C4A-N9A-C8A	2.65	108.52	105.74
3	E	411	COA	C5A-N7A-C8A	2.64	107.60	103.45
2	B	410	FAD	C4X-C10-N1	-2.61	118.19	124.59
3	B	411	COA	C5A-N7A-C8A	2.60	107.54	103.45
2	E	410	FAD	C4X-C10-N1	-2.59	118.24	124.59
2	D	410	FAD	C4X-C10-N1	-2.59	118.25	124.59
3	F	411	COA	C5A-N7A-C8A	2.59	107.51	103.45
2	A	410	FAD	C5A-N7A-C8A	2.58	107.50	103.45
2	B	410	FAD	C5A-N7A-C8A	2.55	107.46	103.45
2	D	410	FAD	C4-C4X-N5	2.55	121.73	118.21
2	C	410	FAD	C5A-N7A-C8A	2.55	107.46	103.45
3	A	411	COA	C5A-N7A-C8A	2.55	107.45	103.45
2	A	410	FAD	C4X-C10-N1	-2.54	118.36	124.59
2	A	410	FAD	C4-C4X-N5	2.52	121.69	118.21
2	F	410	FAD	C5A-N7A-C8A	2.52	107.40	103.45
2	E	410	FAD	C5A-N7A-C8A	2.51	107.40	103.45
3	D	411	COA	C5A-N7A-C8A	2.49	107.36	103.45
2	F	410	FAD	C4X-C10-N1	-2.47	118.53	124.59
2	D	410	FAD	C5A-N7A-C8A	2.46	107.31	103.45
2	C	410	FAD	C4X-C10-N1	-2.43	118.64	124.59
2	D	410	FAD	O4-C4-C4X	-2.30	120.47	126.53
2	A	410	FAD	O4-C4-C4X	-2.29	120.47	126.53
2	F	410	FAD	C4X-C10-N10	2.22	119.66	116.48
2	C	410	FAD	O4-C4-C4X	-2.22	120.67	126.53
2	D	410	FAD	C6A-C5A-N7A	2.18	136.30	132.09
2	E	410	FAD	C10-N1-C2	2.18	121.58	116.85
2	B	410	FAD	C10-N1-C2	2.18	121.56	116.85
2	B	410	FAD	C6A-C5A-N7A	2.17	136.28	132.09
3	E	411	COA	C6A-C5A-N7A	2.16	136.26	132.09
3	F	411	COA	C6A-C5A-N7A	2.15	136.24	132.09
2	A	410	FAD	C4X-C10-N10	2.15	119.57	116.48
2	A	410	FAD	N9A-C8A-N7A	-2.15	110.89	113.94
2	C	410	FAD	C4X-C10-N10	2.15	119.56	116.48
2	A	410	FAD	C6A-C5A-N7A	2.15	136.23	132.09
2	F	410	FAD	C10-N1-C2	2.14	121.49	116.85
3	B	411	COA	C6A-C5A-N7A	2.14	136.21	132.09
3	A	411	COA	C6A-C5A-N7A	2.14	136.21	132.09
2	B	410	FAD	C4X-C10-N10	2.14	119.54	116.48
2	D	410	FAD	C10-N1-C2	2.14	121.47	116.85
2	E	410	FAD	O4-C4-C4X	-2.13	120.90	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	410	FAD	N9A-C8A-N7A	-2.13	110.91	113.94
2	A	410	FAD	C10-N1-C2	2.12	121.44	116.85
2	F	410	FAD	C6A-C5A-N7A	2.11	136.17	132.09
2	B	410	FAD	O4-C4-C4X	-2.11	120.95	126.53
3	E	411	COA	O6A-CCP-CBP	-2.11	107.16	110.55
2	F	410	FAD	O4-C4-C4X	-2.10	120.98	126.53
2	E	410	FAD	C6A-C5A-N7A	2.10	136.13	132.09
2	D	410	FAD	C4X-C10-N10	2.09	119.48	116.48
2	E	410	FAD	C4X-C10-N10	2.09	119.47	116.48
3	E	411	COA	C3B-C2B-C1B	2.08	104.47	99.89
3	B	411	COA	N9A-C8A-N7A	-2.08	110.98	113.94
3	E	411	COA	N9A-C8A-N7A	-2.08	110.99	113.94
3	D	411	COA	C7P-C6P-C5P	-2.07	108.94	112.39
2	F	410	FAD	C4X-C4-N3	2.07	118.53	113.25
2	C	410	FAD	C6A-C5A-N7A	2.06	136.06	132.09
3	F	411	COA	N9A-C8A-N7A	-2.06	111.02	113.94
2	C	410	FAD	C10-N1-C2	2.06	121.30	116.85
3	A	411	COA	N9A-C8A-N7A	-2.05	111.03	113.94
2	D	410	FAD	C4X-C4-N3	2.05	118.47	113.25
2	E	410	FAD	C4X-C4-N3	2.05	118.46	113.25
3	D	411	COA	C6A-C5A-N7A	2.04	136.03	132.09
3	D	411	COA	N9A-C8A-N7A	-2.04	111.04	113.94
2	B	410	FAD	C4X-C4-N3	2.04	118.45	113.25
2	D	410	FAD	N9A-C8A-N7A	-2.03	111.06	113.94
2	A	410	FAD	C4X-C4-N3	2.03	118.42	113.25
2	F	410	FAD	N9A-C8A-N7A	-2.03	111.06	113.94
2	C	410	FAD	C4X-C4-N3	2.02	118.40	113.25
2	B	410	FAD	N9A-C8A-N7A	-2.02	111.07	113.94
2	F	410	FAD	C4'-C3'-C2'	-2.01	110.22	113.57
2	D	410	FAD	C4-N3-C2	-2.00	122.08	125.64

There are no chirality outliers.

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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'
2	B	410	FAD	C5B-O5B-PA-O2A
2	B	410	FAD	C5B-O5B-PA-O3P
2	B	410	FAD	C2'-C3'-C4'-O4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	C	410	FAD	C5B-O5B-PA-O2A
2	C	410	FAD	C5B-O5B-PA-O3P
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'
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	E	410	FAD	C5B-O5B-PA-O2A
2	E	410	FAD	C5B-O5B-PA-O3P
2	F	410	FAD	C5B-O5B-PA-O2A
2	F	410	FAD	C5B-O5B-PA-O3P
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'
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	B	411	COA	C5B-O5B-P1A-O1A
3	B	411	COA	C5B-O5B-P1A-O3A
3	B	411	COA	CCP-O6A-P2A-O3A
3	B	411	COA	CCP-O6A-P2A-O4A
3	B	411	COA	S1P-C2P-C3P-N4P
3	D	411	COA	CCP-O6A-P2A-O3A
3	E	411	COA	C5B-O5B-P1A-O2A
3	E	411	COA	C5B-O5B-P1A-O3A
3	E	411	COA	CCP-O6A-P2A-O3A
3	E	411	COA	CCP-O6A-P2A-O4A
3	E	411	COA	CCP-O6A-P2A-O5A
3	F	411	COA	C5B-O5B-P1A-O1A
3	F	411	COA	C5B-O5B-P1A-O3A
3	F	411	COA	CCP-O6A-P2A-O3A
3	F	411	COA	CDP-CBP-CCP-O6A
3	F	411	COA	CEP-CBP-CCP-O6A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	411	COA	CAP-CBP-CCP-O6A
3	A	411	COA	O9P-C9P-N8P-C7P
2	A	410	FAD	C2'-C3'-C4'-C5'
2	C	410	FAD	C2'-C3'-C4'-C5'
3	D	411	COA	O4B-C4B-C5B-O5B
2	C	410	FAD	O2'-C2'-C3'-O3'
3	A	411	COA	O4B-C4B-C5B-O5B
3	F	411	COA	O4B-C4B-C5B-O5B
2	C	410	FAD	O2'-C2'-C3'-C4'
3	B	411	COA	O4B-C4B-C5B-O5B
2	E	410	FAD	O3'-C3'-C4'-C5'
2	E	410	FAD	O3'-C3'-C4'-O4'
3	B	411	COA	P1A-O3A-P2A-O6A
3	F	411	COA	P1A-O3A-P2A-O6A
2	C	410	FAD	C1'-C2'-C3'-O3'
2	D	410	FAD	O2'-C2'-C3'-O3'
2	D	410	FAD	O2'-C2'-C3'-C4'
2	E	410	FAD	C2'-C3'-C4'-O4'
2	E	410	FAD	C2'-C3'-C4'-C5'
3	B	411	COA	C3B-C4B-C5B-O5B
3	E	411	COA	P1A-O3A-P2A-O4A
3	F	411	COA	C2P-C3P-N4P-C5P
3	E	411	COA	S1P-C2P-C3P-N4P
2	A	410	FAD	C5B-O5B-PA-O3P
2	B	410	FAD	C5B-O5B-PA-O1A
2	C	410	FAD	C5B-O5B-PA-O1A
2	D	410	FAD	C5B-O5B-PA-O3P
2	E	410	FAD	C5B-O5B-PA-O1A
2	F	410	FAD	C5B-O5B-PA-O1A
3	A	411	COA	CCP-O6A-P2A-O4A
3	B	411	COA	C5B-O5B-P1A-O2A
3	D	411	COA	CCP-O6A-P2A-O4A
3	E	411	COA	C5B-O5B-P1A-O1A
3	F	411	COA	C5B-O5B-P1A-O2A
3	F	411	COA	CCP-O6A-P2A-O4A
3	E	411	COA	P1A-O3A-P2A-O5A
3	E	411	COA	C3B-O3B-P3B-O9A
3	F	411	COA	C3B-O3B-P3B-O9A
3	D	411	COA	C2P-C3P-N4P-C5P
3	D	411	COA	C3B-C4B-C5B-O5B
3	B	411	COA	C4B-C5B-O5B-P1A
2	A	410	FAD	O2'-C2'-C3'-O3'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	410	FAD	C1'-C2'-C3'-O3'
2	D	410	FAD	C1'-C2'-C3'-O3'
2	E	410	FAD	C1'-C2'-C3'-O3'
3	E	411	COA	O4B-C4B-C5B-O5B
2	A	410	FAD	PA-O3P-P-O2P
2	B	410	FAD	PA-O3P-P-O2P
3	A	411	COA	P1A-O3A-P2A-O5A
2	A	410	FAD	O2'-C2'-C3'-C4'
3	A	411	COA	C3B-O3B-P3B-O8A
2	E	410	FAD	O2'-C2'-C3'-O3'
3	A	411	COA	N8P-C9P-CAP-OAP
3	B	411	COA	N8P-C9P-CAP-OAP
3	E	411	COA	N8P-C9P-CAP-OAP
3	F	411	COA	N8P-C9P-CAP-OAP
3	F	411	COA	P1A-O3A-P2A-O5A

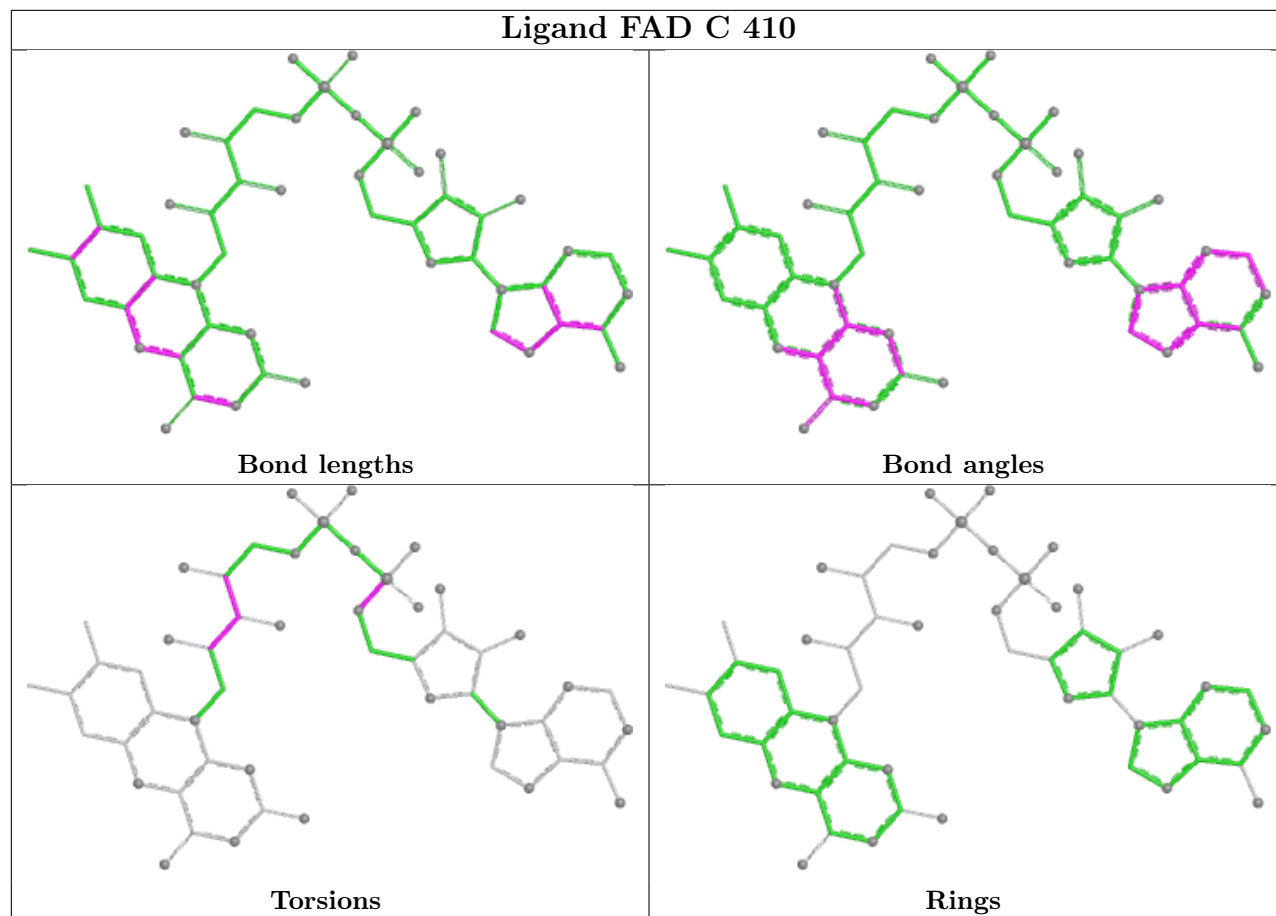
There are no ring outliers.

10 monomers are involved in 14 short contacts:

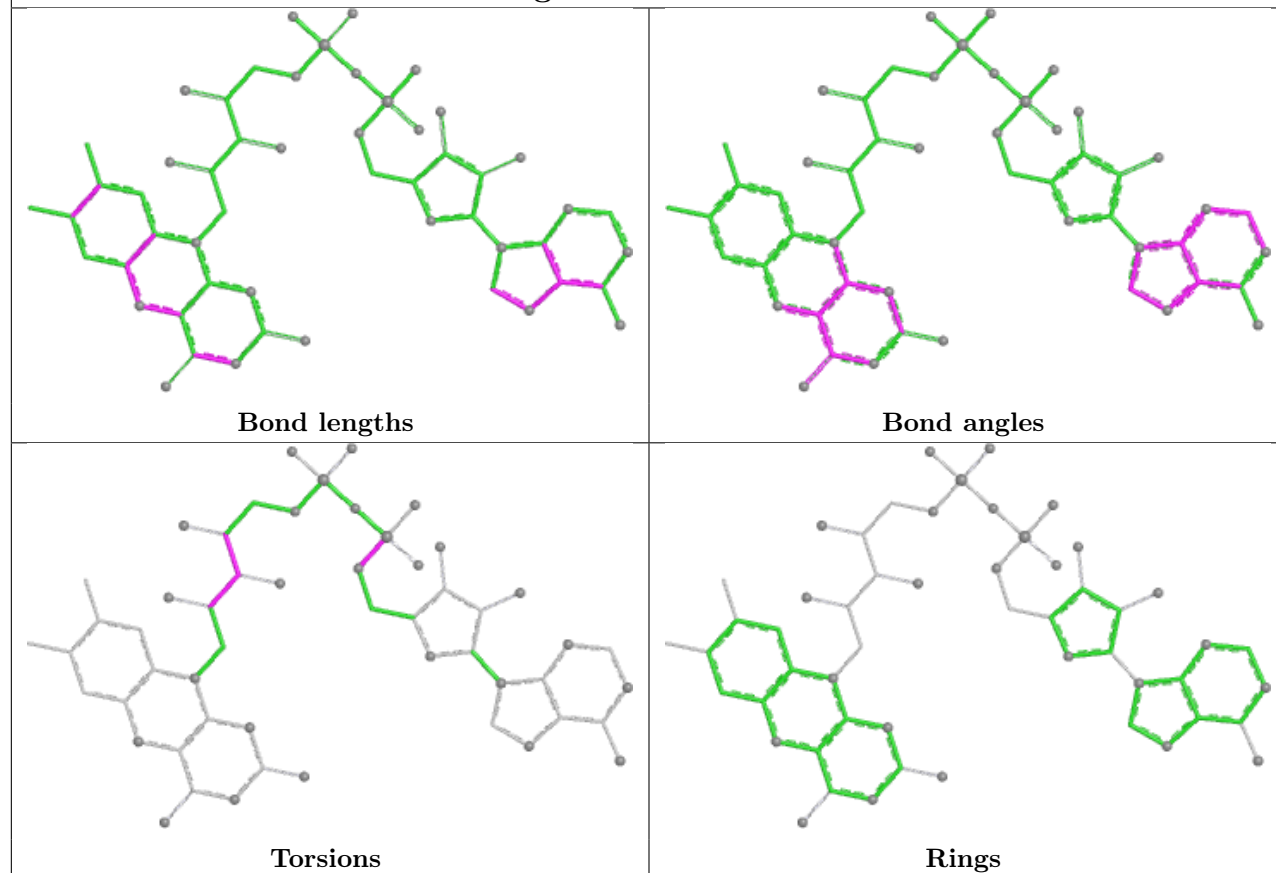
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	410	FAD	1	0
4	C	412	SIN	3	0
3	F	411	COA	2	0
2	F	410	FAD	3	0
2	A	410	FAD	1	0
2	D	410	FAD	2	0
3	E	411	COA	1	0
3	A	411	COA	2	0
3	D	411	COA	3	0
3	B	411	COA	1	0

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

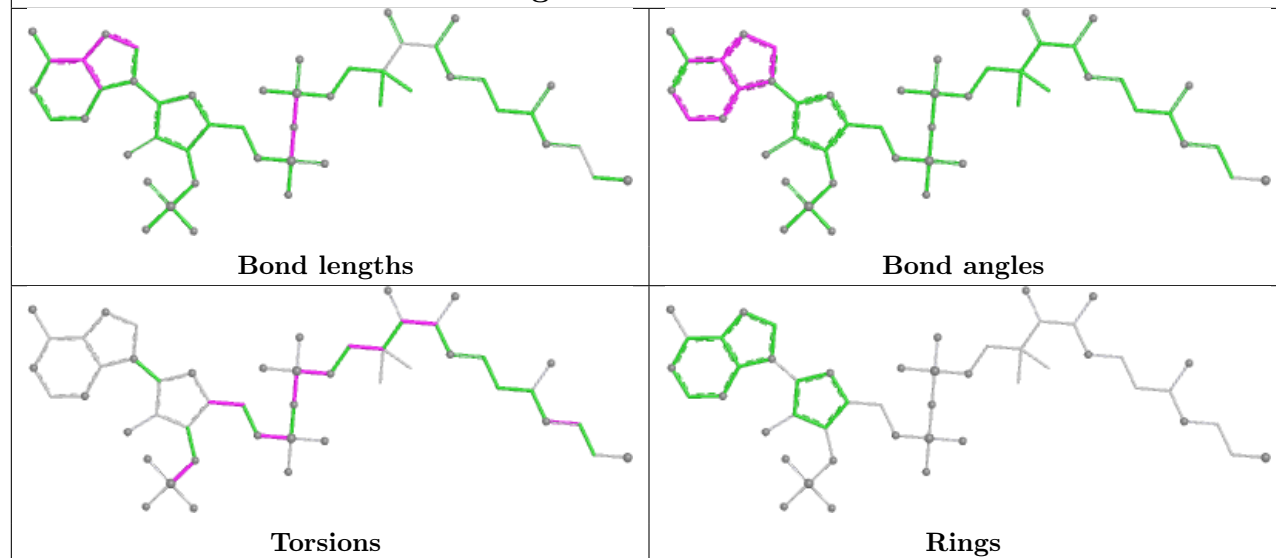
equivalents in the CSD to analyse the geometry.

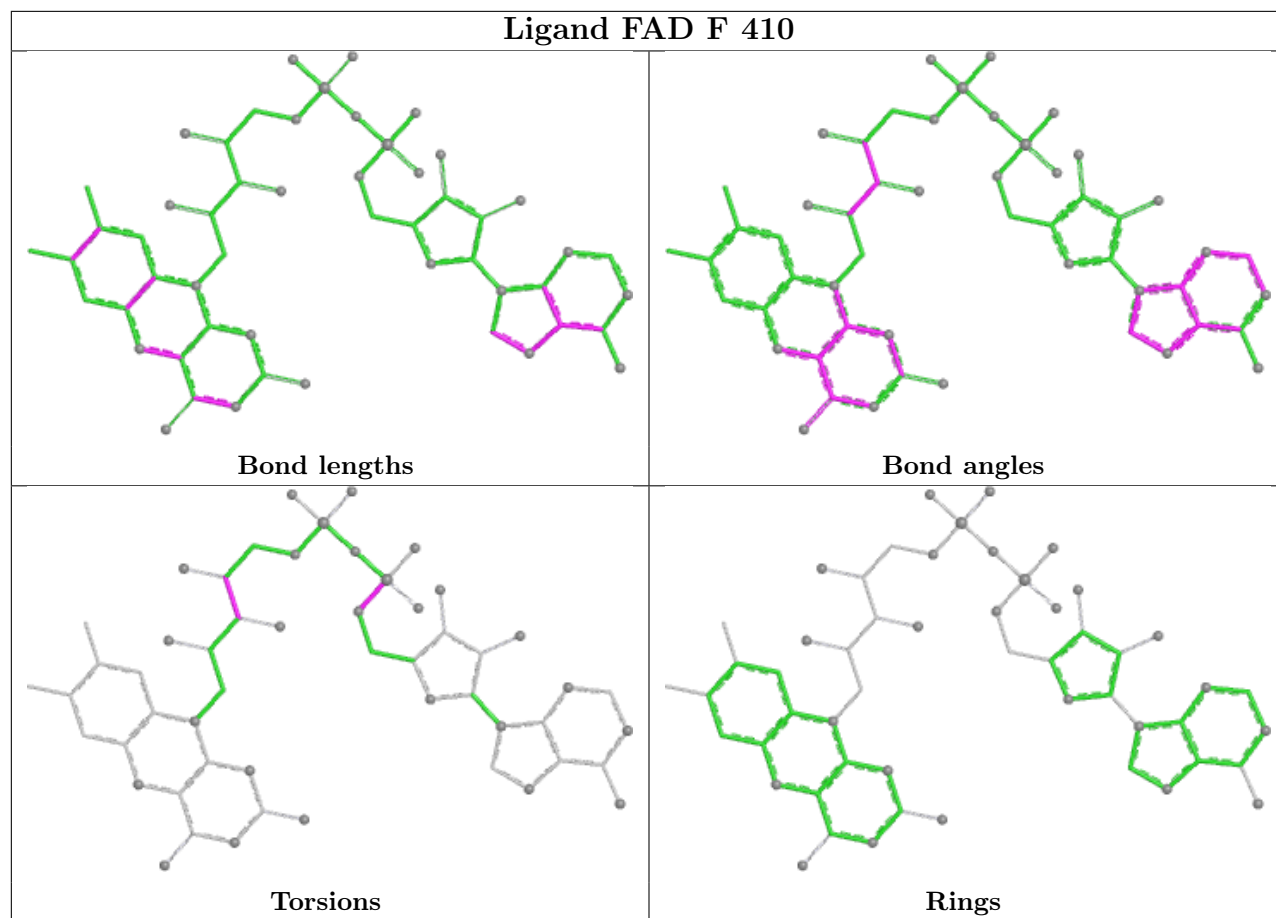


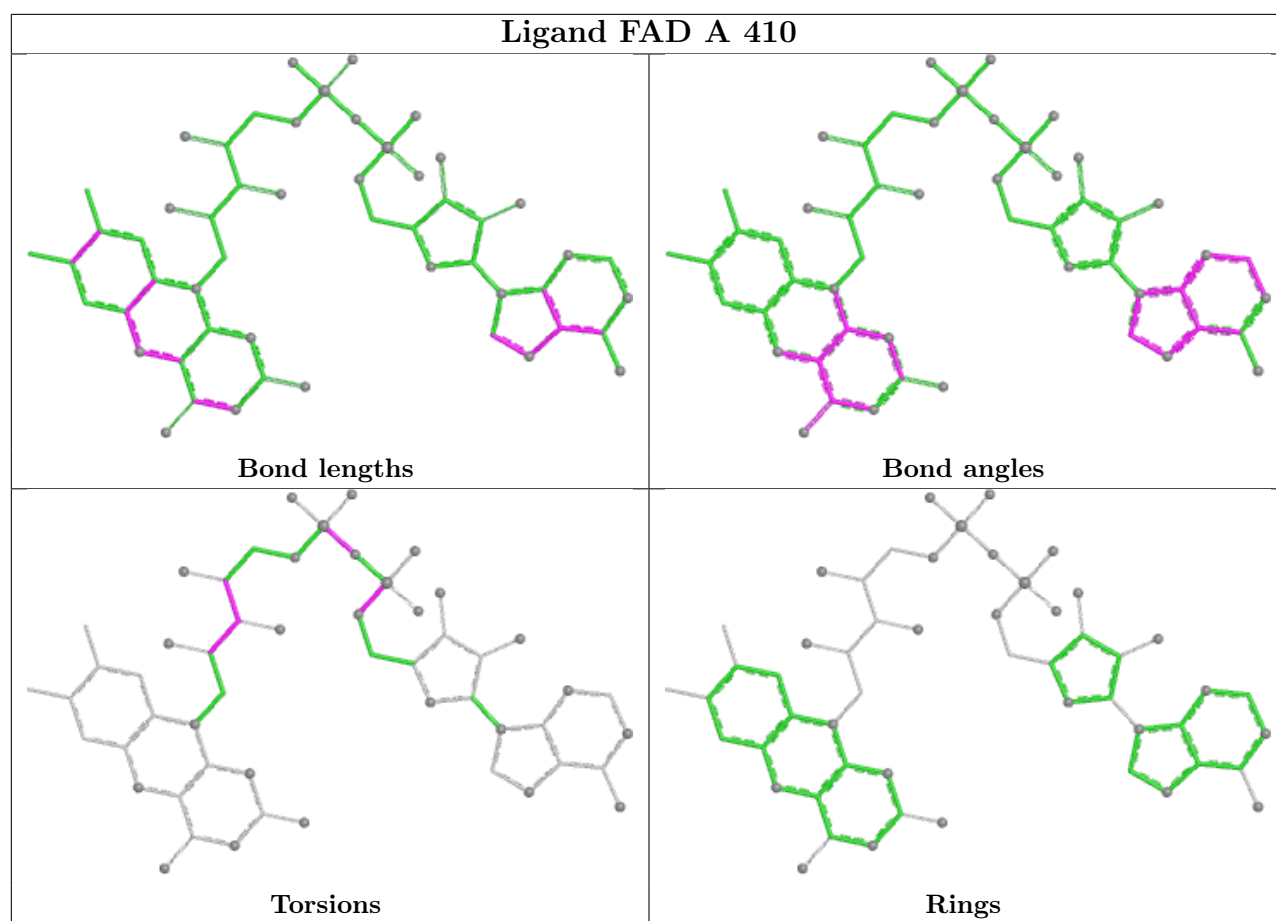
Ligand FAD E 410



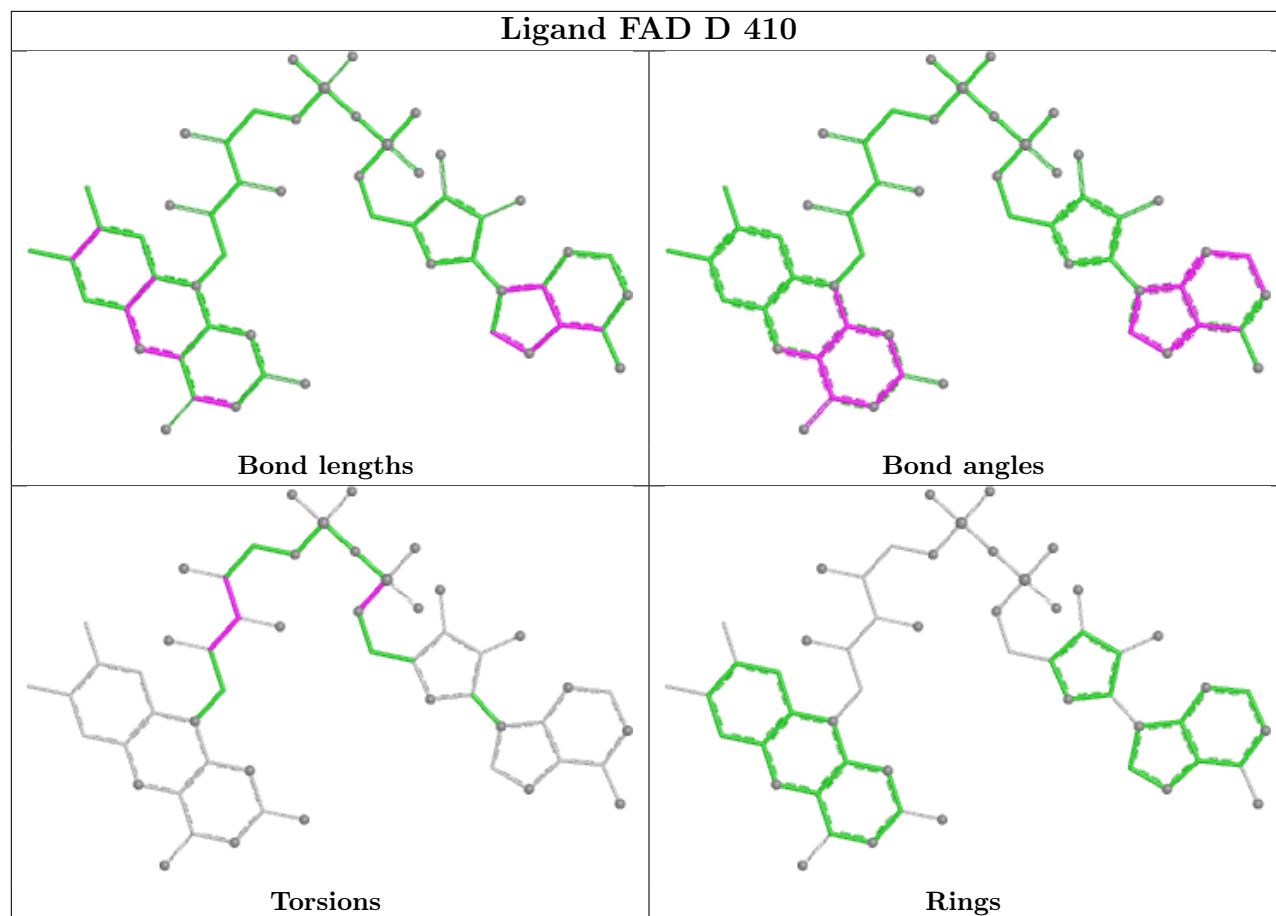
Ligand COA F 411



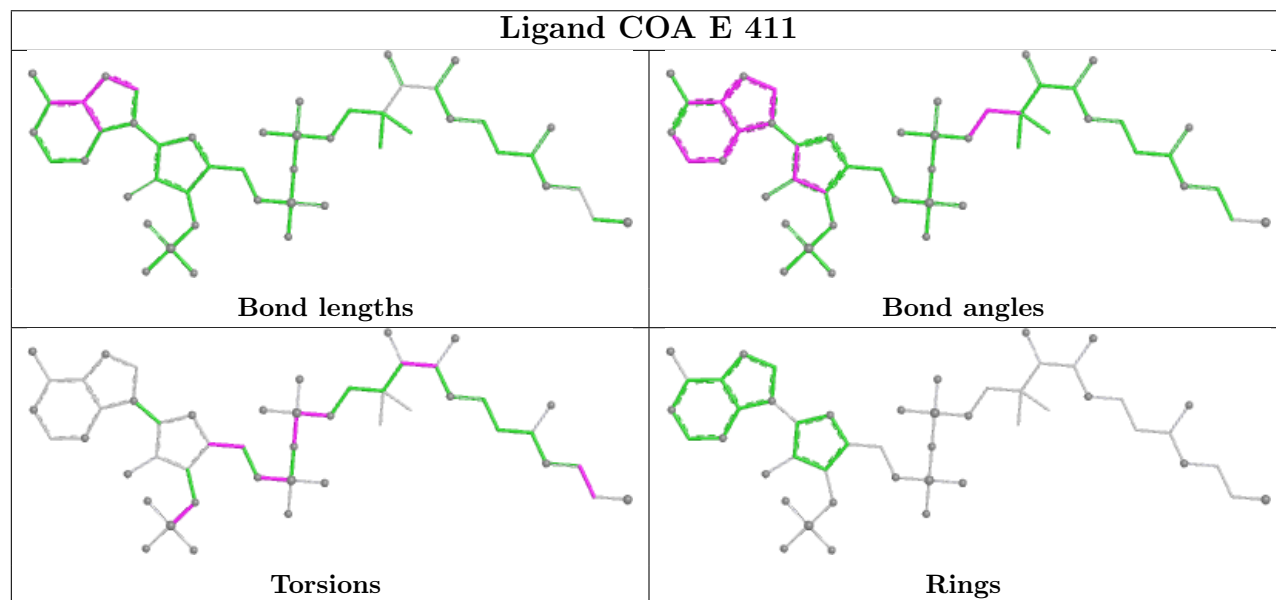




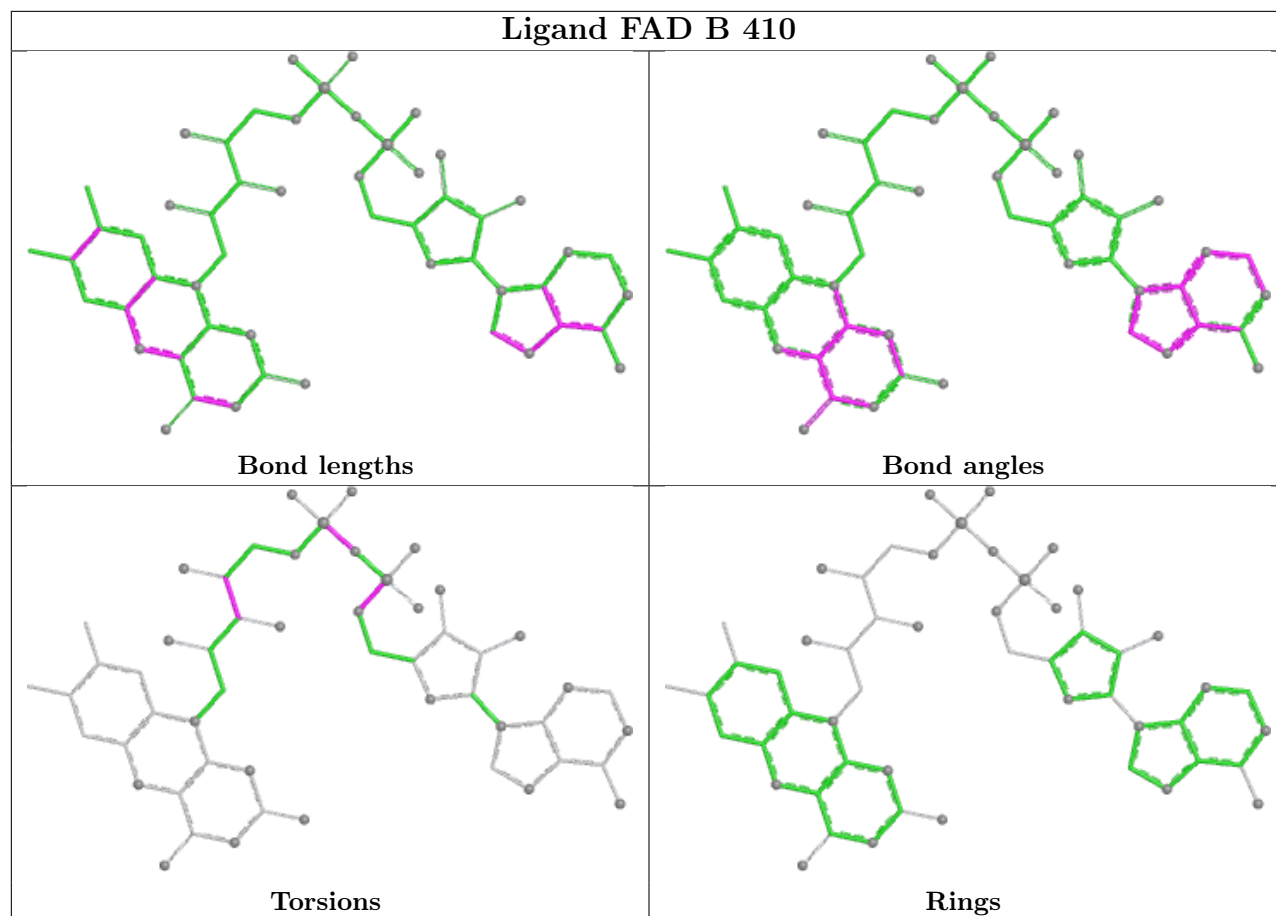
Ligand FAD D 410



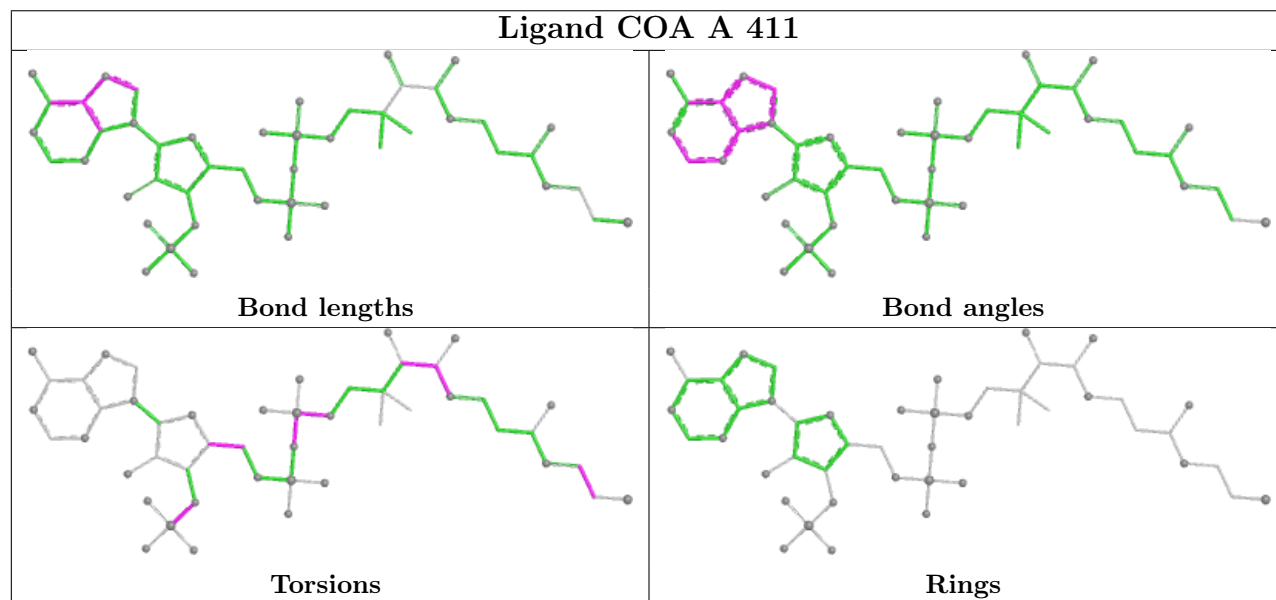
Ligand COA E 411

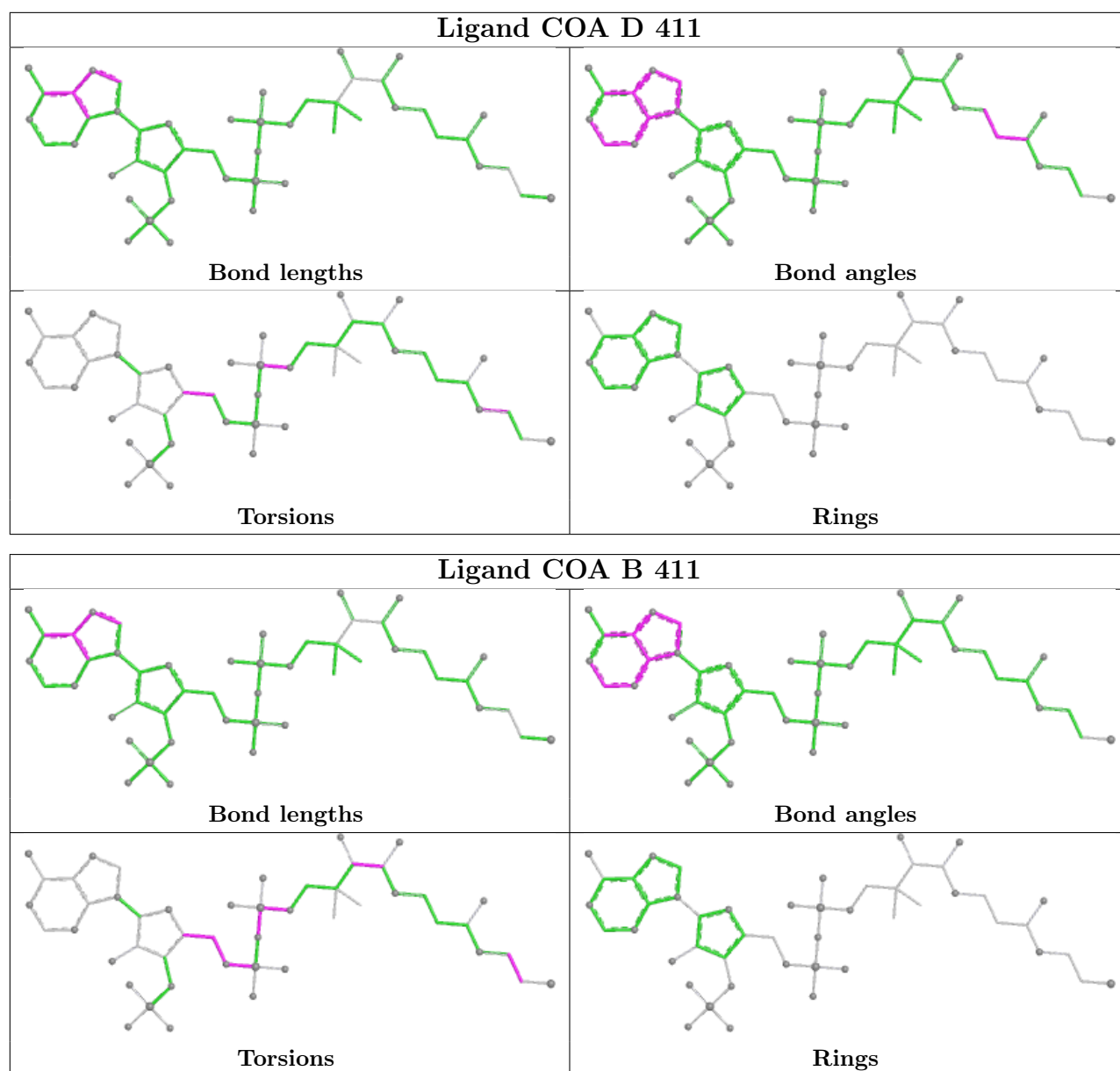


Ligand FAD B 410



Ligand COA A 411





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

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%)	0.11	8 (2%) 65 66	29, 43, 67, 98	1 (0%)
1	B	391/401 (97%)	0.28	24 (6%) 27 29	27, 45, 84, 112	1 (0%)
1	C	391/401 (97%)	0.43	22 (5%) 30 32	31, 50, 81, 104	0
1	D	390/401 (97%)	0.44	13 (3%) 49 51	34, 53, 77, 106	0
1	E	391/401 (97%)	0.87	63 (16%) 4 5	30, 53, 89, 112	0
1	F	391/401 (97%)	1.06	84 (21%) 2 3	30, 58, 101, 119	1 (0%)
All	All	2345/2406 (97%)	0.53	214 (9%) 15 16	27, 50, 89, 119	3 (0%)

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	392	TYR	6.1
1	B	228	PHE	5.1
1	F	228	PHE	5.0
1	E	224	MET	4.9
1	E	239	LEU	4.8
1	F	226	ILE	4.6
1	E	227	THR	4.5
1	C	2	TYR	4.4
1	F	179	ILE	4.4
1	E	392	TYR	4.4
1	F	100	TYR	4.4
1	F	220	ILE	4.4
1	B	231	GLY	4.3
1	C	243	TYR	4.3
1	B	232	LEU	4.3
1	E	97	ILE	4.2
1	C	392	TYR	4.2
1	F	146	TYR	4.1
1	E	232	LEU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	229	PRO	4.0
1	E	139	ALA	3.9
1	D	392	TYR	3.9
1	E	226	ILE	3.9
1	E	236	PHE	3.8
1	F	170	VAL	3.8
1	E	228	PHE	3.8
1	B	392	TYR	3.8
1	F	171	PHE	3.7
1	F	137	THR	3.7
1	E	100	TYR	3.7
1	F	229	PRO	3.7
1	F	236	PHE	3.6
1	F	101	GLY	3.6
1	F	242	ALA	3.6
1	D	229	PRO	3.6
1	B	229	PRO	3.6
1	E	170	VAL	3.6
1	E	237	ALA	3.5
1	F	178	GLY	3.5
1	F	227	THR	3.5
1	C	190	GLY	3.5
1	F	182	PHE	3.5
1	B	100	TYR	3.4
1	C	236	PHE	3.4
1	E	313	PHE	3.4
1	C	231	GLY	3.4
1	F	232	LEU	3.3
1	A	190	GLY	3.2
1	F	121	ILE	3.2
1	F	166	ILE	3.2
1	A	243	TYR	3.2
1	E	2	TYR	3.2
1	F	168	ALA	3.2
1	C	173	ASP	3.2
1	F	230	ASP	3.2
1	D	231	GLY	3.1
1	E	231	GLY	3.1
1	D	232	LEU	3.1
1	F	155	ILE	3.1
1	A	236	PHE	3.1
1	E	178	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	235	GLY	3.0
1	A	392	TYR	3.0
1	F	129	GLY	3.0
1	F	313	PHE	3.0
1	F	113	VAL	2.9
1	F	391	GLY	2.9
1	F	132	ALA	2.9
1	F	148	LEU	2.9
1	E	230	ASP	2.9
1	B	233	LYS	2.9
1	C	230	ASP	2.9
1	C	147	ILE	2.9
1	F	218	LEU	2.8
1	F	237	ALA	2.8
1	B	242	ALA	2.8
1	E	168	ALA	2.8
1	E	171	PHE	2.8
1	F	133	SER	2.8
1	F	109	ALA	2.8
1	F	224	MET	2.8
1	F	193	GLY	2.8
1	F	225	MET	2.8
1	F	175	VAL	2.8
1	E	246	GLN	2.7
1	F	150	GLY	2.7
1	E	215	PHE	2.7
1	E	221	HIS	2.7
1	F	147	ILE	2.7
1	E	93	ALA	2.7
1	F	2	TYR	2.7
1	F	53	MET	2.7
1	F	136	THR	2.7
1	B	122	CYS	2.7
1	F	243	TYR	2.6
1	F	142	ASN	2.6
1	E	220	ILE	2.6
1	E	225	MET	2.6
1	A	2	TYR	2.6
1	C	143	GLY	2.6
1	B	383	MET	2.6
1	C	241	SER	2.6
1	D	189	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	233	LYS	2.6
1	F	122	CYS	2.6
1	F	134	GLU	2.6
1	E	146	TYR	2.6
1	F	388	THR	2.6
1	E	183	ILE	2.6
1	E	240	MET	2.6
1	E	314	PRO	2.6
1	D	243	TYR	2.6
1	F	231	GLY	2.5
1	F	241	SER	2.5
1	D	190	GLY	2.5
1	F	235	GLY	2.5
1	A	246[A]	GLN	2.5
1	B	170	VAL	2.5
1	B	226	ILE	2.5
1	E	243	TYR	2.5
1	E	310	GLY	2.5
1	E	391	GLY	2.5
1	E	98	THR	2.5
1	B	239	LEU	2.5
1	E	104	GLU	2.4
1	D	175	VAL	2.4
1	E	166	ILE	2.4
1	C	172	ASP	2.4
1	E	167	PHE	2.4
1	F	106	ILE	2.4
1	B	188	ASP	2.4
1	B	174	GLY	2.4
1	F	139	ALA	2.4
1	E	179	ILE	2.4
1	E	222	LYS	2.4
1	F	215	PHE	2.4
1	C	232	LEU	2.4
1	A	229	PRO	2.4
1	F	131	ALA	2.4
1	E	182	PHE	2.4
1	F	194	LEU	2.4
1	E	189	HIS	2.4
1	F	189	HIS	2.4
1	B	230	ASP	2.3
1	E	51	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	143	GLY	2.3
1	F	50	MET	2.3
1	B	313	PHE	2.3
1	E	122	CYS	2.3
1	E	188	ASP	2.3
1	C	59	GLY	2.3
1	B	179	ILE	2.3
1	F	386	PRO	2.3
1	E	96	ALA	2.3
1	E	57	SER	2.3
1	F	54	LEU	2.3
1	F	191	PRO	2.3
1	D	276	GLY	2.3
1	E	234	ARG	2.3
1	F	311	GLU	2.3
1	E	147	ILE	2.3
1	F	186	LEU	2.2
1	F	213	LEU	2.2
1	D	172	ASP	2.2
1	E	312	THR	2.2
1	E	148	LEU	2.2
1	F	239	LEU	2.2
1	C	141	LYS	2.2
1	F	102	SER	2.2
1	D	230	ASP	2.2
1	E	235	GLY	2.2
1	F	92	GLY	2.2
1	F	145	HIS	2.2
1	F	181	ALA	2.2
1	F	164	HIS	2.2
1	F	234	ARG	2.1
1	F	94	ILE	2.1
1	F	183	ILE	2.1
1	E	317	ASN	2.1
1	E	49	PHE	2.1
1	A	231	GLY	2.1
1	E	150	GLY	2.1
1	F	95	GLY	2.1
1	F	190	GLY	2.1
1	E	68	THR	2.1
1	E	136	THR	2.1
1	E	181	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	242	ALA	2.1
1	F	96	ALA	2.1
1	D	233	LYS	2.1
1	E	165	LEU	2.1
1	F	97	ILE	2.1
1	F	163	LEU	2.1
1	C	58	VAL	2.1
1	C	225	MET	2.1
1	F	172	ASP	2.1
1	F	180	GLY	2.1
1	B	169	ARG	2.1
1	E	137	THR	2.1
1	F	184	THR	2.1
1	F	108	LEU	2.1
1	C	226	ILE	2.1
1	B	190	GLY	2.1
1	C	391	GLY	2.1
1	B	133	SER	2.0
1	E	223	SER	2.0
1	B	181	ALA	2.0
1	C	224	MET	2.0
1	C	245	ALA	2.0
1	F	120	ALA	2.0
1	E	106	ILE	2.0
1	B	227	THR	2.0
1	D	312	THR	2.0
1	F	63	LEU	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 oligosaccharides in this entry.

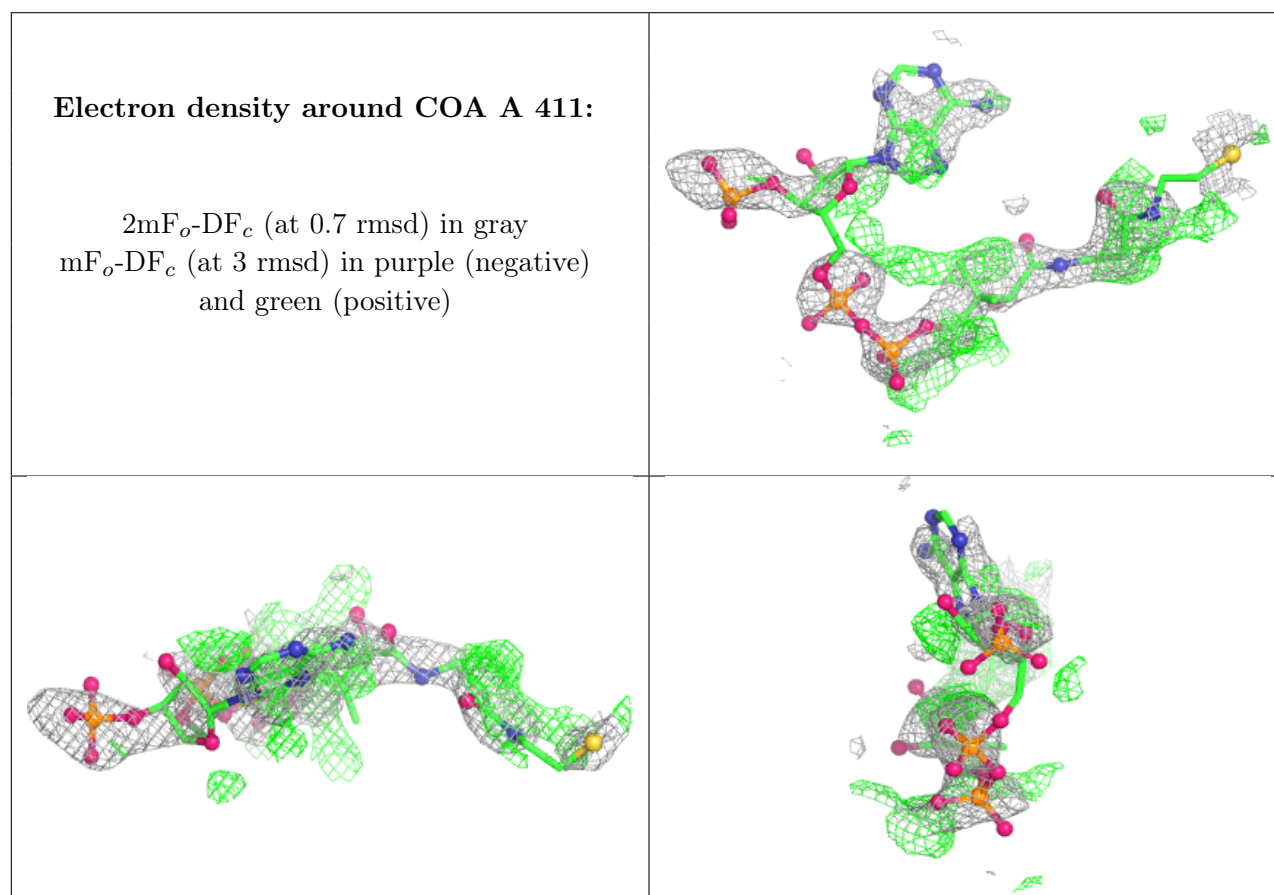
6.4 Ligands [i](#)

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.

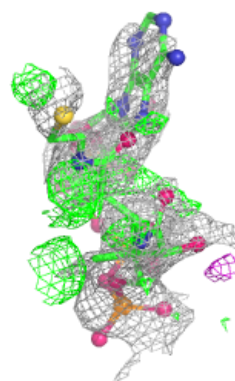
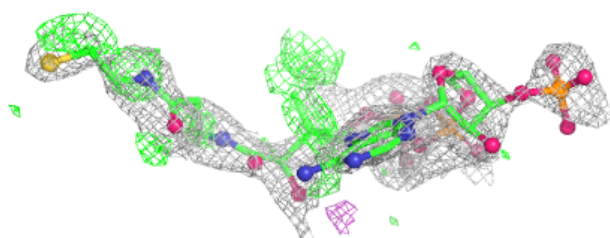
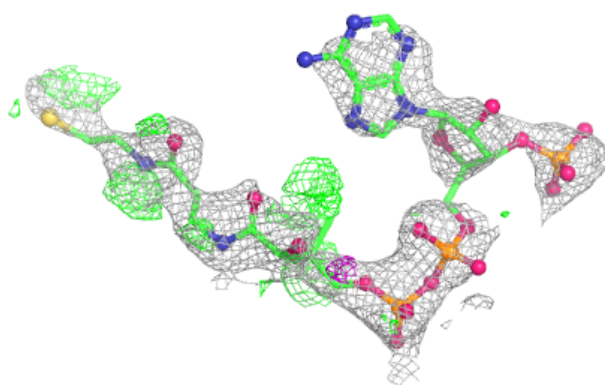
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	COA	A	411	48/48	0.75	0.32	41,56,69,76	48
3	COA	D	411	48/48	0.75	0.22	43,60,75,77	48
3	COA	E	411	48/48	0.77	0.24	58,66,75,91	48
3	COA	B	411	48/48	0.81	0.26	48,60,72,77	48
3	COA	F	411	48/48	0.81	0.23	61,71,79,115	48
5	SO4	C	1393	5/5	0.82	0.14	83,88,102,163	0
4	SIN	C	412	8/8	0.85	0.16	39,60,75,98	0
2	FAD	E	410	53/53	0.92	0.10	35,53,64,68	0
2	FAD	F	410	53/53	0.93	0.10	50,61,77,84	0
2	FAD	B	410	53/53	0.94	0.08	29,42,52,57	0
2	FAD	A	410	53/53	0.95	0.08	26,33,47,51	0
2	FAD	C	410	53/53	0.95	0.09	28,39,52,64	0
2	FAD	D	410	53/53	0.95	0.09	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.

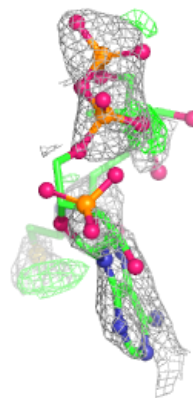
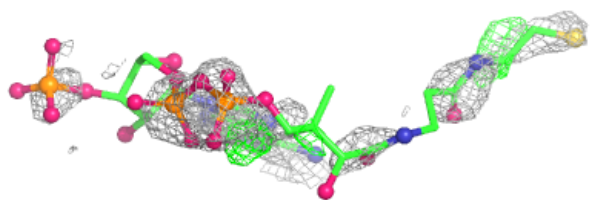
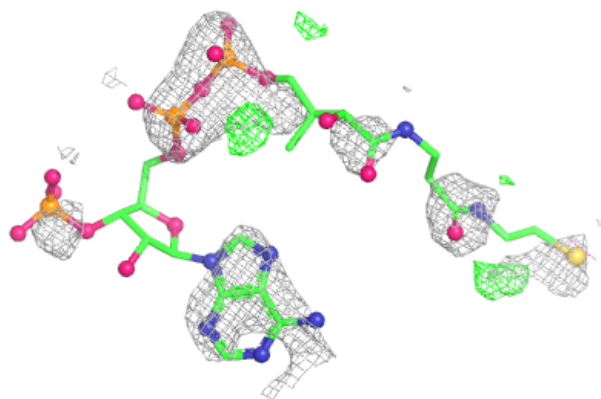


Electron density around COA D 411:

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

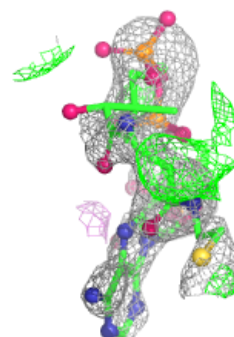
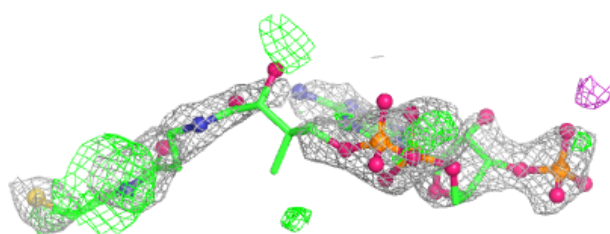
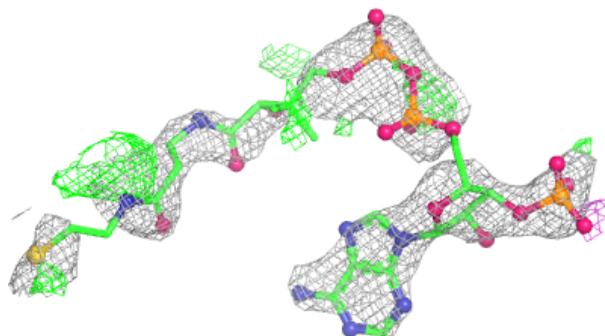
**Electron density around COA E 411:**

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

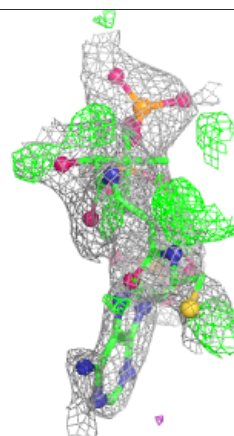
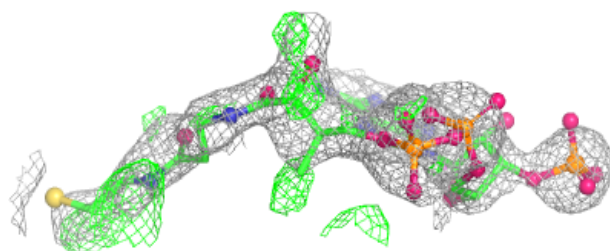
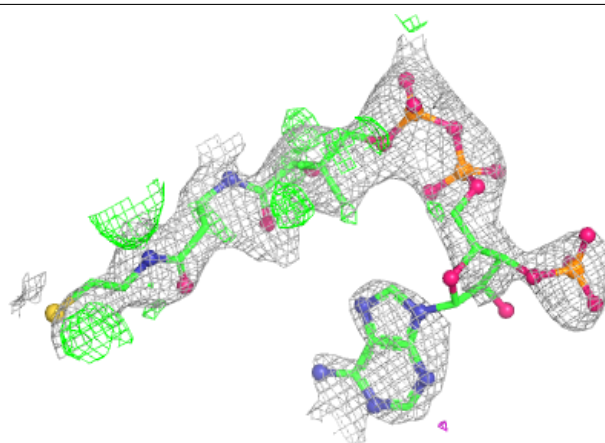


Electron density around COA B 411:

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

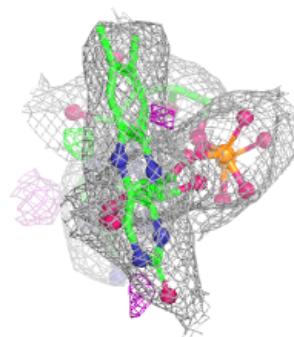
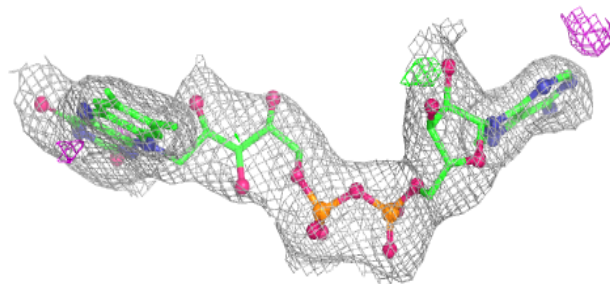
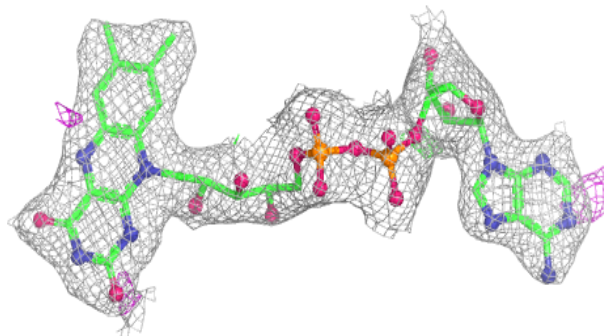
**Electron density around COA F 411:**

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

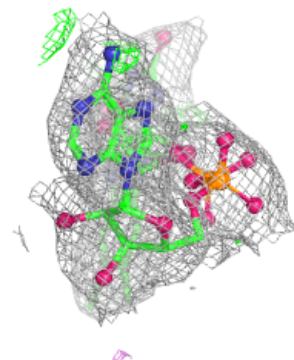
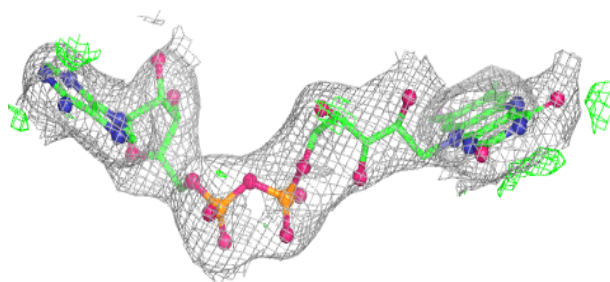
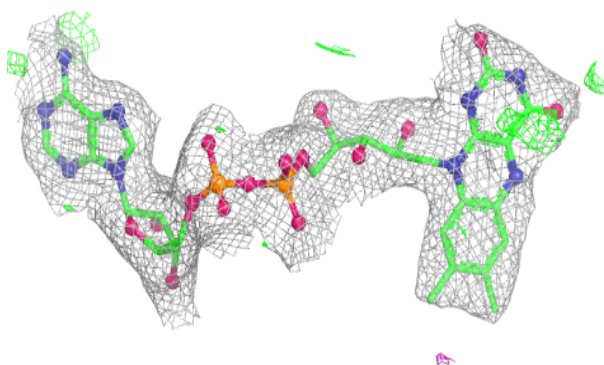


Electron density around FAD E 410:

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

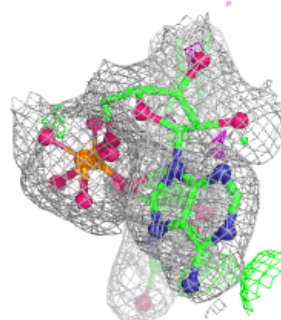
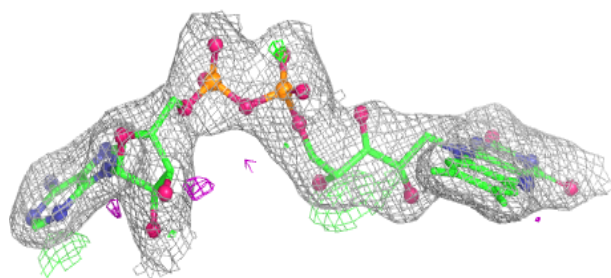
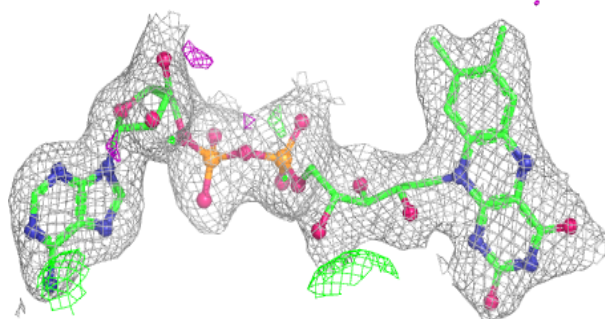
**Electron density around FAD F 410:**

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

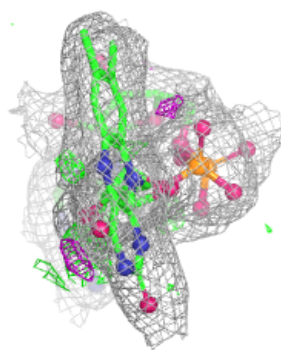
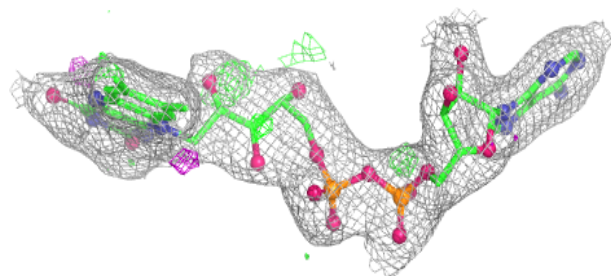
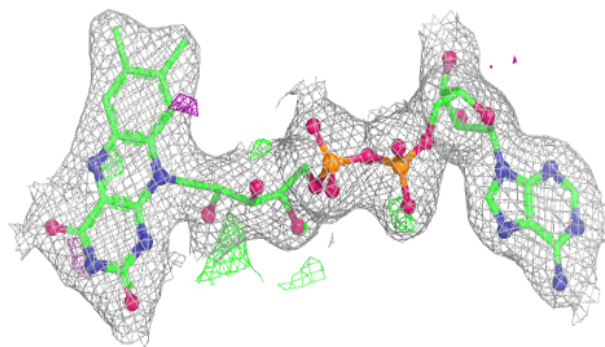


Electron density around FAD B 410:

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

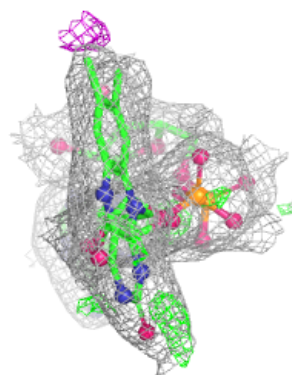
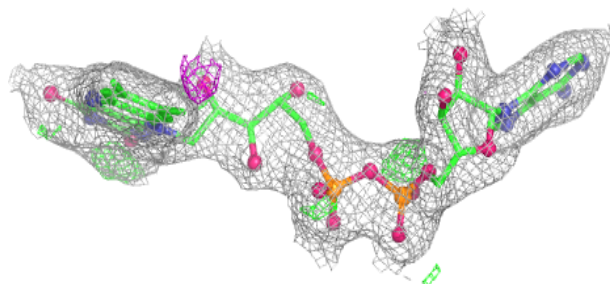
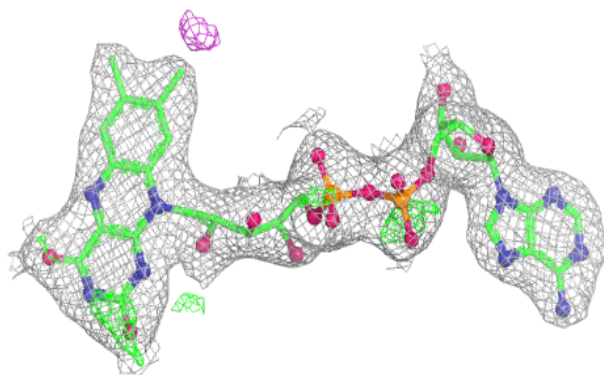
**Electron density around FAD A 410:**

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

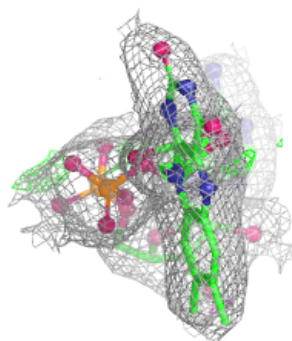
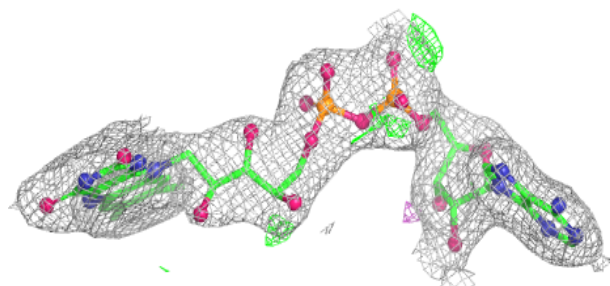
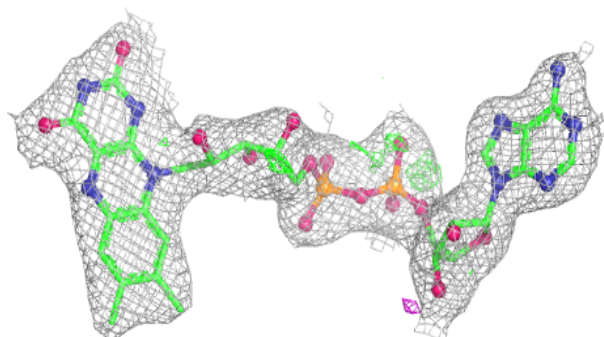


Electron density around FAD C 410:

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

**Electron density around FAD D 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.