



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:36 AM UTC

PDB ID : 4GTE / pdb_00004gte
Title : T. Maritima FDTS (E144R mutant) with FAD and Folate
Authors : Mathews, I.I.; Lesley, S.A.; Kohen, A.; Prabhakar, A.
Deposited on : 2012-08-28
Resolution : 1.89 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

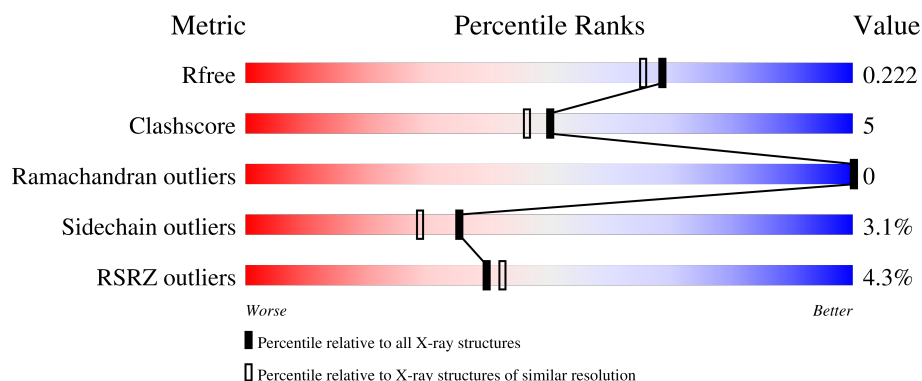
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	232	5% 79% 12% • 7%
1	B	232	5% 80% 11% • 8%
1	C	232	2% 80% 12% • 6%
1	D	232	4% 80% 11% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7627 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 Thymidylate synthase thyX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	1	0
			1815	1180	315	314	6			
1	B	214	Total	C	N	O	S	0	1	0
			1809	1176	313	315	5			
1	C	217	Total	C	N	O	S	0	0	0
			1823	1185	314	319	5			
1	D	214	Total	C	N	O	S	0	2	0
			1807	1177	310	315	5			

There are 52 discrepancies between the modelled and reference sequences:

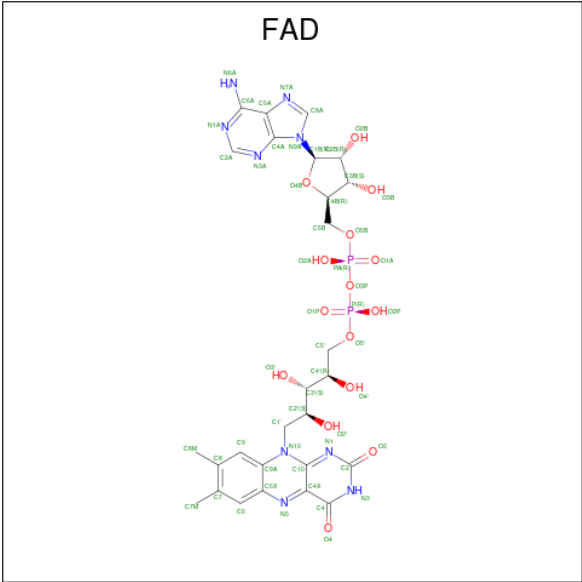
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9WYT0
A	-10	GLY	-	expression tag	UNP Q9WYT0
A	-9	SER	-	expression tag	UNP Q9WYT0
A	-8	ASP	-	expression tag	UNP Q9WYT0
A	-7	LYS	-	expression tag	UNP Q9WYT0
A	-6	ILE	-	expression tag	UNP Q9WYT0
A	-5	HIS	-	expression tag	UNP Q9WYT0
A	-4	HIS	-	expression tag	UNP Q9WYT0
A	-3	HIS	-	expression tag	UNP Q9WYT0
A	-2	HIS	-	expression tag	UNP Q9WYT0
A	-1	HIS	-	expression tag	UNP Q9WYT0
A	0	HIS	-	expression tag	UNP Q9WYT0
A	144	ARG	GLU	engineered mutation	UNP Q9WYT0
B	-11	MET	-	expression tag	UNP Q9WYT0
B	-10	GLY	-	expression tag	UNP Q9WYT0
B	-9	SER	-	expression tag	UNP Q9WYT0
B	-8	ASP	-	expression tag	UNP Q9WYT0
B	-7	LYS	-	expression tag	UNP Q9WYT0
B	-6	ILE	-	expression tag	UNP Q9WYT0
B	-5	HIS	-	expression tag	UNP Q9WYT0
B	-4	HIS	-	expression tag	UNP Q9WYT0

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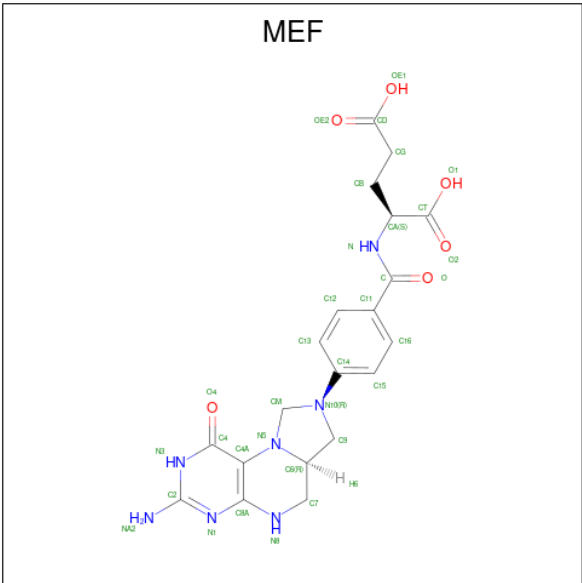
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q9WYT0
B	-2	HIS	-	expression tag	UNP Q9WYT0
B	-1	HIS	-	expression tag	UNP Q9WYT0
B	0	HIS	-	expression tag	UNP Q9WYT0
B	144	ARG	GLU	engineered mutation	UNP Q9WYT0
C	-11	MET	-	expression tag	UNP Q9WYT0
C	-10	GLY	-	expression tag	UNP Q9WYT0
C	-9	SER	-	expression tag	UNP Q9WYT0
C	-8	ASP	-	expression tag	UNP Q9WYT0
C	-7	LYS	-	expression tag	UNP Q9WYT0
C	-6	ILE	-	expression tag	UNP Q9WYT0
C	-5	HIS	-	expression tag	UNP Q9WYT0
C	-4	HIS	-	expression tag	UNP Q9WYT0
C	-3	HIS	-	expression tag	UNP Q9WYT0
C	-2	HIS	-	expression tag	UNP Q9WYT0
C	-1	HIS	-	expression tag	UNP Q9WYT0
C	0	HIS	-	expression tag	UNP Q9WYT0
C	144	ARG	GLU	engineered mutation	UNP Q9WYT0
D	-11	MET	-	expression tag	UNP Q9WYT0
D	-10	GLY	-	expression tag	UNP Q9WYT0
D	-9	SER	-	expression tag	UNP Q9WYT0
D	-8	ASP	-	expression tag	UNP Q9WYT0
D	-7	LYS	-	expression tag	UNP Q9WYT0
D	-6	ILE	-	expression tag	UNP Q9WYT0
D	-5	HIS	-	expression tag	UNP Q9WYT0
D	-4	HIS	-	expression tag	UNP Q9WYT0
D	-3	HIS	-	expression tag	UNP Q9WYT0
D	-2	HIS	-	expression tag	UNP Q9WYT0
D	-1	HIS	-	expression tag	UNP Q9WYT0
D	0	HIS	-	expression tag	UNP Q9WYT0
D	144	ARG	GLU	engineered mutation	UNP Q9WYT0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			35	15	5	13	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
			35	15	5	13	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is N-({4-[(6aR)-3-amino-1-oxo-1,2,5,6,6a,7-hexahydroimidazo[1,5-f]pteridin-8(9H)-yl]phenyl}carbonyl)-L-glutamic acid (CCD ID: MEF) (formula: C₂₀H₂₃N₇O₆).

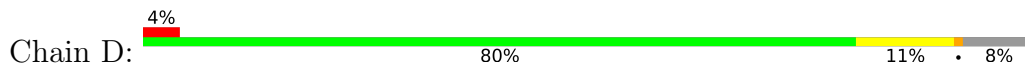


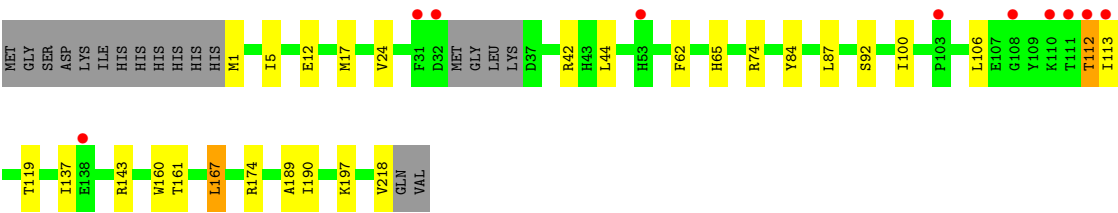
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			15	8	6	1		
3	D	1	Total	C	N	O	0	0
			15	8	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	38	Total	O	0	1
			39	39		
4	C	42	Total	O	0	3
			45	45		
4	D	40	Total	O	0	1
			41	41		

- Molecule 1: Thymidylate synthase thyX





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.71Å 117.07Å 141.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.47 – 1.89 38.47 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.47-1.89) 99.2 (38.47-1.89)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.184 , 0.213 0.192 , 0.222	Depositor DCC
R_{free} test set	3719 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7627	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: MEF, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	3/1869 (0.2%)	0.97	0/2525
1	B	0.98	1/1857 (0.1%)	0.94	0/2509
1	C	0.99	1/1871 (0.1%)	0.98	1/2527 (0.0%)
1	D	0.95	0/1862	0.91	0/2517
All	All	1.00	5/7459 (0.1%)	0.95	1/10078 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	154	LEU	C-O	-6.12	1.16	1.23
1	A	183	ILE	CA-CB	5.94	1.62	1.54
1	A	137	ILE	CA-CB	5.39	1.60	1.54
1	B	114	PRO	CA-C	5.32	1.54	1.51
1	A	68	ALA	CA-CB	5.21	1.61	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	ILE	N-CA-C	5.42	116.20	110.72

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	1815	0	1806	21	0
1	B	1809	0	1798	20	0
1	C	1823	0	1822	19	0
1	D	1807	0	1807	20	0
2	A	35	0	20	3	0
2	B	53	0	31	2	0
2	C	35	0	20	1	0
2	D	53	0	31	2	0
3	B	15	0	11	0	0
3	D	15	0	11	1	0
4	A	42	0	0	0	0
4	B	39	0	0	0	0
4	C	45	0	0	2	0
4	D	41	0	0	0	0
All	All	7627	0	7357	78	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 5.

All (78) 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:B:89:GLY:HA2	1:B:94:LEU:HD21	1.23	1.11
1:A:173:LEU:HD13	2:A:301:FAD:O4'	1.73	0.87
1:A:17:MET:HB2	1:B:17:MET:HB2	1.57	0.84
1:B:89:GLY:CA	1:B:94:LEU:HD21	2.07	0.80
1:B:89:GLY:HA2	1:B:94:LEU:CD2	2.10	0.80
1:C:28:ARG:HH22	1:C:40:ARG:HD3	1.52	0.74
1:C:219:GLN:O	1:C:220:VAL:HG22	1.88	0.72
1:C:17:MET:HB2	1:D:17:MET:HB2	1.74	0.69
1:C:137:ILE:HD12	1:C:143:ARG:HG3	1.74	0.69
1:B:219:GLN:O	1:B:220:VAL:HG22	1.95	0.66
1:A:137:ILE:HD12	1:A:143:ARG:HG3	1.79	0.64
1:B:94:LEU:HD22	1:B:94:LEU:N	2.12	0.64
1:A:163:ASN:C	1:A:163:ASN:HD22	2.06	0.62
1:B:105:ARG:HG3	1:B:106:LEU:HD13	1.81	0.62
1:C:28:ARG:NH2	1:C:40:ARG:HD3	2.14	0.61
1:A:127:ASP:OD2	1:A:131:ARG:NH1	2.35	0.59
1:B:5:ILE:HD11	1:B:189:ALA:HB2	1.84	0.58
1:D:167[B]:LEU:HD11	1:D:190:ILE:HG21	1.86	0.57
1:D:1:MET:HE1	1:D:197:LYS:HE2	1.88	0.55
1:D:174:ARG:HH22	3:D:302:MEF:HNA2	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:HD11	1:C:189:ALA:HB2	1.89	0.54
1:D:112:THR:HG22	1:D:113:ILE:HG23	1.90	0.53
1:A:173:LEU:HD13	2:A:301:FAD:HO4'	1.70	0.53
1:A:163:ASN:ND2	1:A:166:SER:H	2.07	0.52
1:C:55:THR:HG23	4:C:438:HOH:O	2.09	0.52
1:A:137:ILE:CD1	1:A:143:ARG:HG3	2.40	0.51
1:D:87:LEU:HD11	1:D:92:SER:OG	2.11	0.51
1:B:25:ARG:HG3	1:B:30:SER:O	2.11	0.51
1:B:94:LEU:CD2	1:B:94:LEU:N	2.75	0.49
1:B:102:SER:O	1:B:105:ARG:HB3	2.12	0.49
1:A:145:VAL:HG11	1:D:106:LEU:HD11	1.93	0.49
1:B:173:LEU:HD13	2:B:301:FAD:O4'	2.12	0.49
1:D:167[B]:LEU:HD11	1:D:190:ILE:CG2	2.42	0.49
1:C:116:GLU:CD	1:C:116:GLU:H	2.21	0.48
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.96	0.48
1:A:165:ARG:CZ	2:C:301:FAD:H2B	2.44	0.48
1:C:117:ARG:NH2	4:C:436:HOH:O	2.47	0.47
1:C:30:SER:OG	1:C:32:ASP:HB2	2.15	0.47
1:A:102:SER:O	1:A:105:ARG:HB3	2.14	0.47
1:C:167:LEU:C	1:C:167:LEU:HD23	2.40	0.47
2:A:301:FAD:H2B	1:C:165:ARG:CZ	2.45	0.47
1:C:137:ILE:CD1	1:C:143:ARG:HG3	2.43	0.46
1:A:192:ARG:HH11	1:A:192:ARG:CG	2.29	0.46
1:D:24:VAL:HG13	1:D:44:LEU:HD23	1.98	0.45
1:B:116:GLU:H	1:B:116:GLU:CD	2.25	0.45
1:A:106:LEU:HD13	1:A:118:VAL:HG11	1.98	0.45
1:B:112:THR:HG22	1:B:112:THR:O	2.16	0.45
1:A:188:LEU:HD23	1:A:215:LEU:HD23	1.99	0.44
1:B:175:ALA:HA	1:B:214:ILE:HD11	1.99	0.44
1:C:102:SER:O	1:C:105:ARG:HB3	2.17	0.44
1:B:104:GLU:HA	1:B:107:GLU:HG2	1.99	0.44
1:D:137:ILE:HD11	1:D:143:ARG:HA	1.99	0.44
1:C:219:GLN:HG3	1:C:220:VAL:HG13	1.98	0.44
1:A:21:LEU:HD13	1:A:33:MET:HA	1.99	0.44
1:D:84:TYR:CE2	1:D:160:TRP:CD1	3.06	0.44
1:B:192:ARG:HD3	1:B:220:VAL:HG21	2.01	0.43
2:B:301:FAD:H9	2:B:301:FAD:H1'1	1.85	0.43
1:A:163:ASN:C	1:A:163:ASN:ND2	2.75	0.43
1:D:100:ILE:HG22	1:D:119:THR:HG23	2.00	0.43
1:C:5:ILE:HG22	1:C:6:LEU:HG	1.99	0.43
1:B:127:ASP:O	1:B:131:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ILE:HD11	1:B:143:ARG:HA	2.00	0.42
2:D:301:FAD:O4'	2:D:301:FAD:H1'1	2.20	0.42
1:D:87:LEU:CD1	1:D:92:SER:OG	2.67	0.42
1:B:140:GLY:C	1:C:111:THR:HG22	2.45	0.42
1:C:84:TYR:CE2	1:C:160:TRP:CD1	3.08	0.41
1:D:62:PHE:O	1:D:161:THR:HA	2.19	0.41
1:D:112:THR:O	1:D:112:THR:CG2	2.63	0.41
1:D:12:GLU:HG2	1:D:65:HIS:HB3	2.02	0.41
1:A:122:ILE:O	1:A:126:VAL:HG23	2.20	0.41
1:C:93:LYS:HD3	1:C:94:LEU:N	2.34	0.41
1:A:126:VAL:HG21	1:A:153:ASN:HD21	1.86	0.41
1:A:55:THR:N	1:A:56:PRO:CD	2.84	0.40
1:A:74:ARG:HG2	1:D:74:ARG:CD	2.51	0.40
1:D:1:MET:HE3	1:D:1:MET:HB2	1.88	0.40
1:D:5:ILE:HD11	1:D:189:ALA:HB2	2.03	0.40
2:D:301:FAD:H1'1	2:D:301:FAD:H9	1.97	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	212/232 (91%)	206 (97%)	6 (3%)	0	100	100
1	B	209/232 (90%)	201 (96%)	8 (4%)	0	100	100
1	C	213/232 (92%)	208 (98%)	5 (2%)	0	100	100
1	D	212/232 (91%)	206 (97%)	6 (3%)	0	100	100
All	All	846/928 (91%)	821 (97%)	25 (3%)	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	193/207 (93%)	188 (97%)	5 (3%)	40	35
1	B	192/207 (93%)	186 (97%)	6 (3%)	35	29
1	C	194/207 (94%)	185 (95%)	9 (5%)	24	16
1	D	193/207 (93%)	188 (97%)	5 (3%)	40	35
All	All	772/828 (93%)	747 (97%)	25 (3%)	35	27

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	107	GLU
1	A	143	ARG
1	A	163	ASN
1	A	192	ARG
1	B	25	ARG
1	B	106	LEU
1	B	110	LYS
1	B	116	GLU
1	B	117	ARG
1	B	135	GLU
1	C	40	ARG
1	C	87	LEU
1	C	93	LYS
1	C	104	GLU
1	C	110	LYS
1	C	117	ARG
1	C	138	GLU
1	C	143	ARG
1	C	217	GLU
1	D	42	ARG
1	D	112	THR
1	D	167[A]	LEU
1	D	167[B]	LEU
1	D	218	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	85	ASN
1	A	163	ASN
1	B	219	GLN
1	C	85	ASN
1	D	85	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	D	301	-	58,58,58	3.06	18 (31%)	85,89,89	1.76	23 (27%)
3	MEF	B	302	-	13,17,36	2.34	4 (30%)	13,25,52	4.02	7 (53%)
2	FAD	B	301	-	58,58,58	3.16	21 (36%)	85,89,89	1.86	22 (25%)
2	FAD	A	301	-	37,37,58	1.82	6 (16%)	53,56,89	1.81	14 (26%)
3	MEF	D	302	-	13,17,36	2.51	4 (30%)	13,25,52	4.61	9 (69%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	C	301	-	37,37,58	1.73	6 (16%)	53,56,89	1.69	11 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	301	-	-	2/34/50/50	0/6/6/6
3	MEF	B	302	-	-	-	0/3/3/4
2	FAD	B	301	-	-	7/34/50/50	0/6/6/6
2	FAD	A	301	-	-	2/30/46/50	0/3/3/6
3	MEF	D	302	-	-	-	0/3/3/4
2	FAD	C	301	-	-	6/30/46/50	0/3/3/6

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	FAD	C6-C7	10.28	1.53	1.39
2	B	301	FAD	C6-C5X	8.90	1.53	1.40
2	D	301	FAD	C6-C7	8.53	1.51	1.39
2	D	301	FAD	C9A-C5X	7.77	1.53	1.41
2	D	301	FAD	C10-N1	7.43	1.48	1.33
3	D	302	MEF	O4-C4	7.22	1.37	1.23
2	D	301	FAD	C9-C9A	6.97	1.50	1.39
3	B	302	MEF	O4-C4	6.96	1.36	1.23
2	D	301	FAD	C6-C5X	6.91	1.50	1.40
2	A	301	FAD	P-O3P	6.66	1.66	1.59
2	B	301	FAD	C10-N1	6.61	1.46	1.33
2	B	301	FAD	C9-C9A	6.56	1.50	1.39
2	D	301	FAD	C4X-N5	6.39	1.44	1.30
2	B	301	FAD	C9A-C5X	6.32	1.51	1.41
2	B	301	FAD	C4X-N5	6.21	1.44	1.30
2	D	301	FAD	P-O3P	5.72	1.65	1.59
2	B	301	FAD	C9A-N10	-5.65	1.31	1.41
2	C	301	FAD	C5A-C4A	5.65	1.49	1.39
2	C	301	FAD	PA-O3P	5.42	1.65	1.59
2	B	301	FAD	C5A-C4A	5.41	1.48	1.39
2	A	301	FAD	C5A-C4A	5.33	1.48	1.39
2	D	301	FAD	C5A-C4A	5.32	1.48	1.39
2	D	301	FAD	C9A-N10	-5.14	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	FAD	C10-N10	4.87	1.47	1.37
2	B	301	FAD	C10-N10	4.74	1.47	1.37
2	B	301	FAD	C8-C7	4.33	1.51	1.40
2	B	301	FAD	PA-O3P	4.12	1.63	1.59
2	B	301	FAD	P-O3P	3.92	1.63	1.59
2	B	301	FAD	C2-N1	-3.87	1.27	1.36
3	D	302	MEF	CM-N5	3.82	1.48	1.45
2	A	301	FAD	PA-O3P	3.81	1.63	1.59
2	D	301	FAD	C2-N1	-3.77	1.28	1.36
2	D	301	FAD	C8-C7	3.72	1.49	1.40
2	D	301	FAD	PA-O3P	3.38	1.63	1.59
3	B	302	MEF	CM-N5	3.21	1.47	1.45
2	C	301	FAD	C8A-N7A	3.12	1.37	1.31
2	C	301	FAD	P-O3P	2.93	1.62	1.59
2	D	301	FAD	C5X-N5	2.90	1.44	1.39
2	D	301	FAD	C4A-N9A	-2.86	1.31	1.37
2	A	301	FAD	C4A-N9A	-2.85	1.31	1.37
2	D	301	FAD	C4-N3	-2.74	1.33	1.38
2	B	301	FAD	C2A-N1A	2.72	1.38	1.33
2	B	301	FAD	C5X-N5	2.65	1.44	1.39
2	D	301	FAD	C4X-C10	2.64	1.51	1.44
3	D	302	MEF	C4A-N5	2.61	1.44	1.37
2	C	301	FAD	PA-O1A	2.55	1.59	1.50
2	C	301	FAD	C4A-N9A	-2.50	1.32	1.37
3	B	302	MEF	C4A-N5	2.43	1.44	1.37
2	A	301	FAD	PA-O1A	2.39	1.59	1.50
2	B	301	FAD	PA-O1A	2.32	1.58	1.50
2	B	301	FAD	C9-C8	-2.30	1.36	1.39
2	B	301	FAD	C5A-N7A	-2.28	1.34	1.39
2	B	301	FAD	C8A-N7A	2.27	1.36	1.31
3	D	302	MEF	C6-N5	2.20	1.51	1.47
2	B	301	FAD	C5'-C4'	2.11	1.54	1.51
2	D	301	FAD	O2-C2	-2.10	1.20	1.24
2	B	301	FAD	C4A-N9A	-2.10	1.33	1.37
3	B	302	MEF	C6-N5	2.03	1.51	1.47
2	A	301	FAD	C2A-N1A	2.02	1.37	1.33

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	MEF	N10-CM-N5	12.49	109.24	102.92
3	B	302	MEF	N10-CM-N5	10.85	108.41	102.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	MEF	C4A-C4-N3	5.39	120.43	110.94
3	B	302	MEF	C4A-C4-N3	5.35	120.35	110.94
3	D	302	MEF	C2-N1-C8A	5.12	122.39	113.36
2	B	301	FAD	C4-C4X-N5	5.11	125.27	118.21
2	B	301	FAD	C5A-C4A-N3A	-4.83	120.07	126.72
3	D	302	MEF	NA2-C2-N3	4.67	126.61	116.76
2	A	301	FAD	N3A-C2A-N1A	-4.65	121.55	128.58
3	B	302	MEF	C2-N1-C8A	4.62	121.52	113.36
2	B	301	FAD	N3A-C4A-N9A	4.59	134.97	127.17
2	B	301	FAD	N3A-C2A-N1A	-4.42	121.89	128.58
2	A	301	FAD	C4A-N9A-C8A	4.38	110.34	105.74
2	A	301	FAD	C5A-C4A-N3A	-4.34	120.74	126.72
2	D	301	FAD	C5A-C4A-N3A	-4.32	120.77	126.72
2	D	301	FAD	N3A-C4A-N9A	4.29	134.47	127.17
2	D	301	FAD	C4A-N9A-C8A	4.26	110.21	105.74
2	C	301	FAD	N3A-C2A-N1A	-4.03	122.49	128.58
2	C	301	FAD	C5A-C4A-N3A	-4.02	121.19	126.72
2	D	301	FAD	N3A-C2A-N1A	-3.93	122.63	128.58
2	A	301	FAD	N3A-C4A-N9A	3.93	133.85	127.17
2	B	301	FAD	C4X-C10-N1	-3.61	115.73	124.59
2	C	301	FAD	O2A-PA-O1A	3.53	128.88	112.44
2	D	301	FAD	C4X-C10-N1	-3.50	116.01	124.59
3	B	302	MEF	NA2-C2-N3	3.49	124.13	116.76
2	C	301	FAD	C4A-N9A-C8A	3.46	109.37	105.74
2	C	301	FAD	N3A-C4A-N9A	3.41	132.97	127.17
2	D	301	FAD	O4-C4-C4X	-3.31	117.80	126.53
2	B	301	FAD	O4-C4-C4X	-3.26	117.94	126.53
2	B	301	FAD	C4A-N9A-C8A	3.21	109.11	105.74
2	A	301	FAD	C4A-C5A-N7A	-3.21	106.92	110.58
3	B	302	MEF	O4-C4-C4A	-3.09	120.04	127.62
2	C	301	FAD	C1'-C2'-C3'	3.03	115.83	112.11
2	B	301	FAD	C9A-C9-C8	3.01	125.28	119.22
2	C	301	FAD	C2A-N1A-C6A	3.01	123.67	118.73
2	B	301	FAD	O2'-C2'-C3'	3.00	116.27	109.25
2	A	301	FAD	O2A-PA-O1A	2.99	126.35	112.44
3	D	302	MEF	C2-N3-C4	-2.98	119.70	125.11
3	D	302	MEF	NA2-C2-N1	-2.98	113.86	119.67
2	A	301	FAD	C1'-C2'-C3'	2.98	115.76	112.11
2	B	301	FAD	C10-N1-C2	2.97	123.28	116.85
2	C	301	FAD	O2'-C2'-C3'	-2.96	104.87	109.77
2	B	301	FAD	C2A-N1A-C6A	2.93	123.54	118.73
3	D	302	MEF	C8A-C4A-N5	-2.93	115.86	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FAD	C10-C4X-N5	-2.90	118.89	124.81
2	B	301	FAD	C5X-C9A-N10	2.89	120.58	117.97
3	D	302	MEF	O4-C4-C4A	-2.88	120.55	127.62
2	D	301	FAD	C5X-C9A-N10	2.87	120.56	117.97
3	B	302	MEF	C2-N3-C4	-2.78	120.06	125.11
2	B	301	FAD	O2A-PA-O1A	2.77	125.35	112.44
2	A	301	FAD	C2A-N1A-C6A	2.73	123.21	118.73
2	A	301	FAD	C2A-N3A-C4A	2.71	118.46	111.83
2	D	301	FAD	C2A-N1A-C6A	2.69	123.16	118.73
2	B	301	FAD	C2A-N3A-C4A	2.68	118.37	111.83
2	D	301	FAD	C8M-C8-C7	-2.65	115.34	120.76
2	B	301	FAD	C2B-C1B-N9A	2.63	119.85	113.30
2	C	301	FAD	C4A-C5A-N7A	-2.63	107.57	110.58
2	D	301	FAD	N3-C2-N1	2.61	125.06	119.50
2	B	301	FAD	O2-C2-N1	-2.57	117.53	121.80
2	D	301	FAD	C2A-N3A-C4A	2.53	118.02	111.83
2	B	301	FAD	C4X-C4-N3	2.49	119.58	113.25
2	D	301	FAD	C4A-C5A-N7A	-2.46	107.76	110.58
2	D	301	FAD	C4-C4X-N5	2.46	121.61	118.21
2	A	301	FAD	O3P-P-O1P	2.40	117.94	110.70
2	D	301	FAD	C9-C9A-C5X	-2.40	115.78	120.03
2	D	301	FAD	O2-C2-N1	-2.40	117.82	121.80
2	A	301	FAD	C2B-C1B-N9A	2.38	119.21	113.30
2	B	301	FAD	N10-C10-N1	2.37	125.49	118.51
2	A	301	FAD	O2A-PA-O3P	-2.35	100.91	107.27
2	B	301	FAD	C4A-C5A-N7A	-2.35	107.89	110.58
2	B	301	FAD	C9-C9A-C5X	-2.29	115.98	120.03
2	C	301	FAD	C2A-N3A-C4A	2.27	117.37	111.83
2	A	301	FAD	N9A-C8A-N7A	-2.26	110.73	113.94
2	B	301	FAD	C9A-C5X-N5	-2.24	120.08	122.45
2	D	301	FAD	C1'-C2'-C3'	2.21	115.65	109.66
2	D	301	FAD	O2A-PA-O1A	2.20	122.69	112.44
2	D	301	FAD	O4-C4-N3	2.18	124.22	120.11
2	D	301	FAD	C4X-C10-N10	2.15	119.56	116.48
2	D	301	FAD	C5X-N5-C4X	-2.13	114.64	118.09
2	D	301	FAD	N9A-C8A-N7A	-2.11	110.94	113.94
2	C	301	FAD	C2B-C1B-N9A	2.10	118.52	113.30
3	D	302	MEF	N3-C2-N1	-2.07	119.53	123.32
3	B	302	MEF	NA2-C2-N1	-2.07	115.63	119.67
2	D	301	FAD	C9A-C9-C8	2.06	123.36	119.22
2	A	301	FAD	C6A-C5A-N7A	2.04	136.02	132.09
2	D	301	FAD	N10-C10-N1	2.01	124.42	118.51

There are no chirality outliers.

All (17) torsion outliers are listed below:

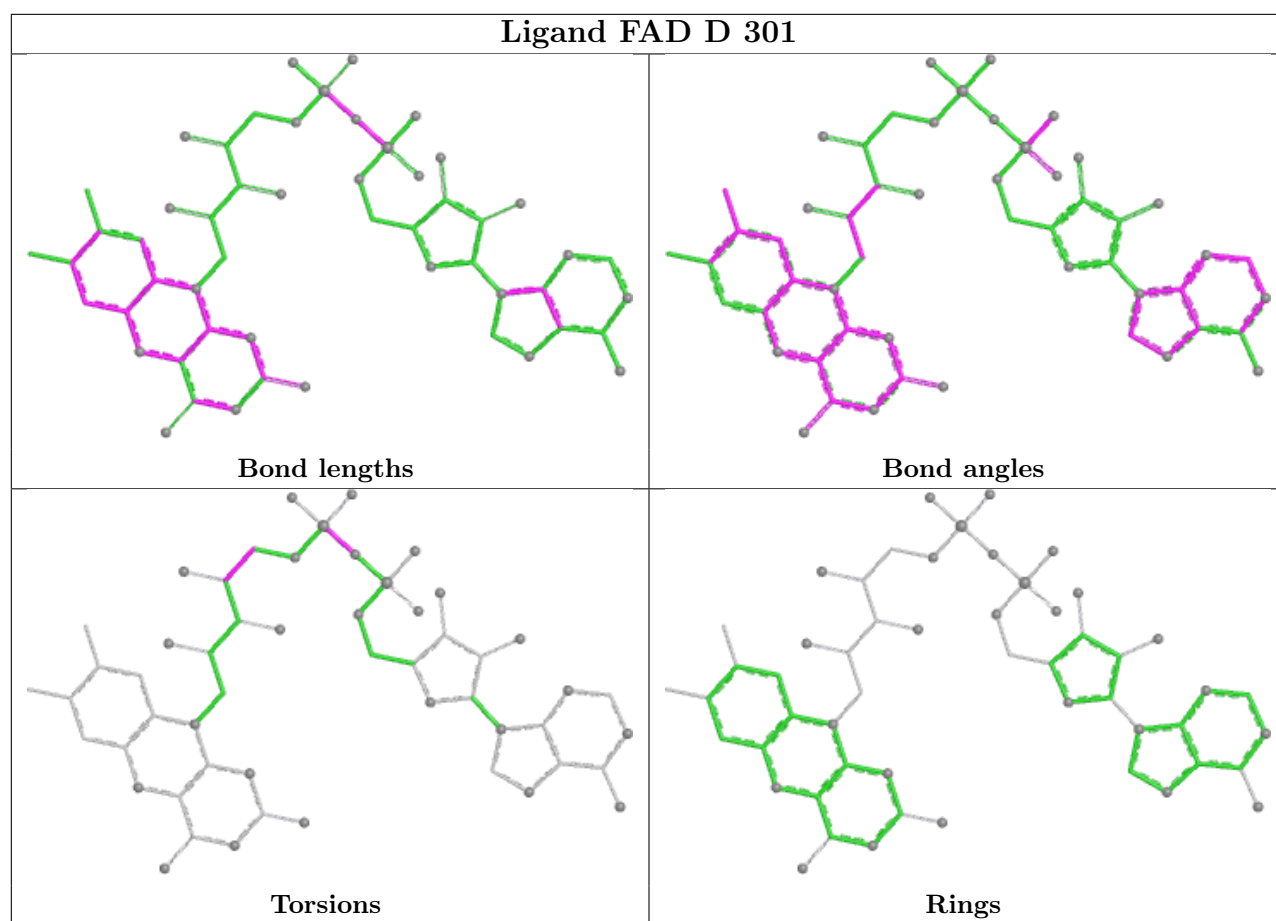
Mol	Chain	Res	Type	Atoms
2	A	301	FAD	C3'-C4'-C5'-O5'
2	A	301	FAD	O4'-C4'-C5'-O5'
2	B	301	FAD	P-O3P-PA-O5B
2	B	301	FAD	C1'-C2'-C3'-O3'
2	B	301	FAD	C1'-C2'-C3'-C4'
2	B	301	FAD	O2'-C2'-C3'-O3'
2	B	301	FAD	O2'-C2'-C3'-C4'
2	B	301	FAD	C3'-C4'-C5'-O5'
2	B	301	FAD	O4'-C4'-C5'-O5'
2	C	301	FAD	C3'-C4'-C5'-O5'
2	C	301	FAD	O4'-C4'-C5'-O5'
2	C	301	FAD	O2'-C2'-C3'-O3'
2	C	301	FAD	C1'-C2'-C3'-O3'
2	C	301	FAD	O2'-C2'-C3'-C4'
2	C	301	FAD	C1'-C2'-C3'-C4'
2	D	301	FAD	O4'-C4'-C5'-O5'
2	D	301	FAD	PA-O3P-P-O2P

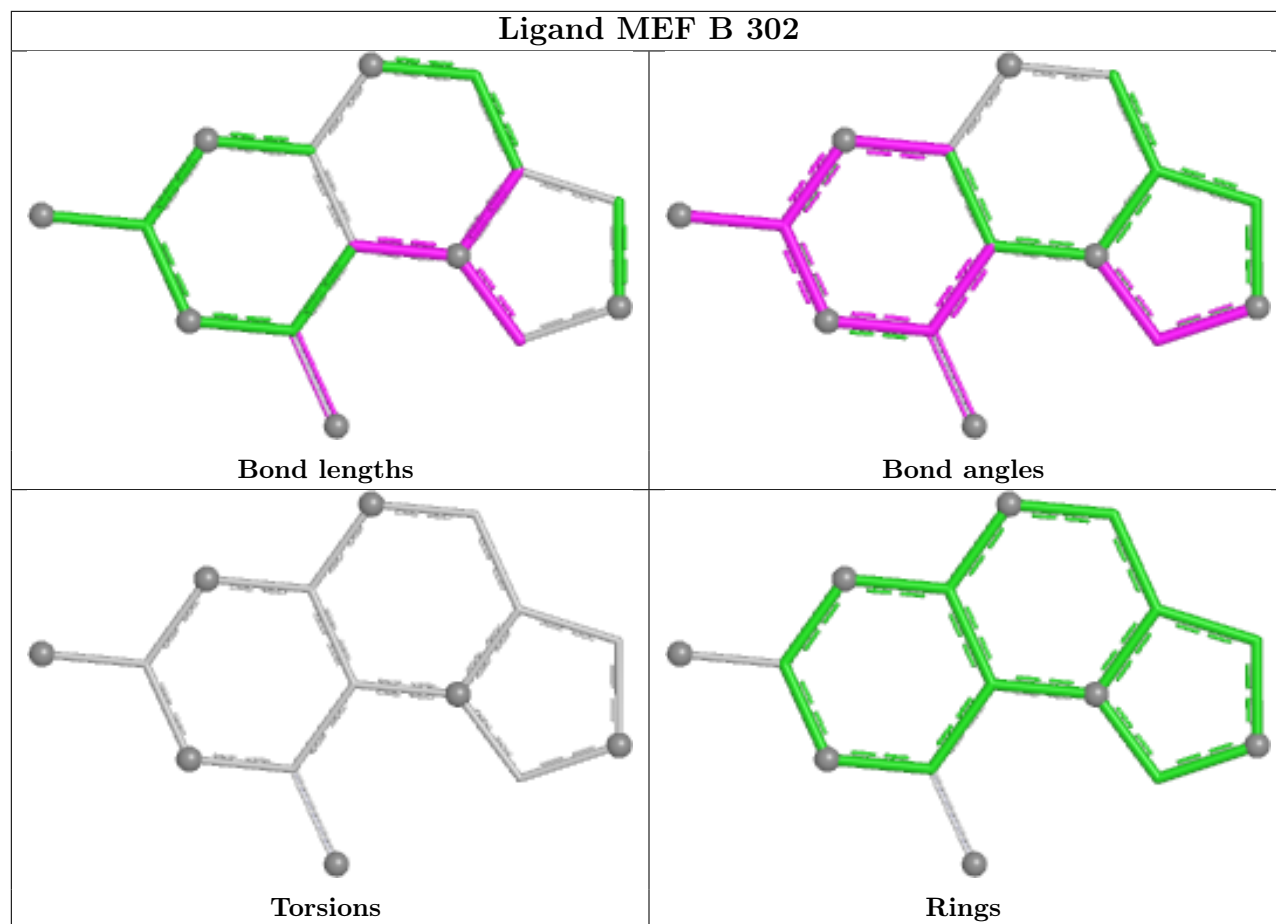
There are no ring outliers.

5 monomers are involved in 9 short contacts:

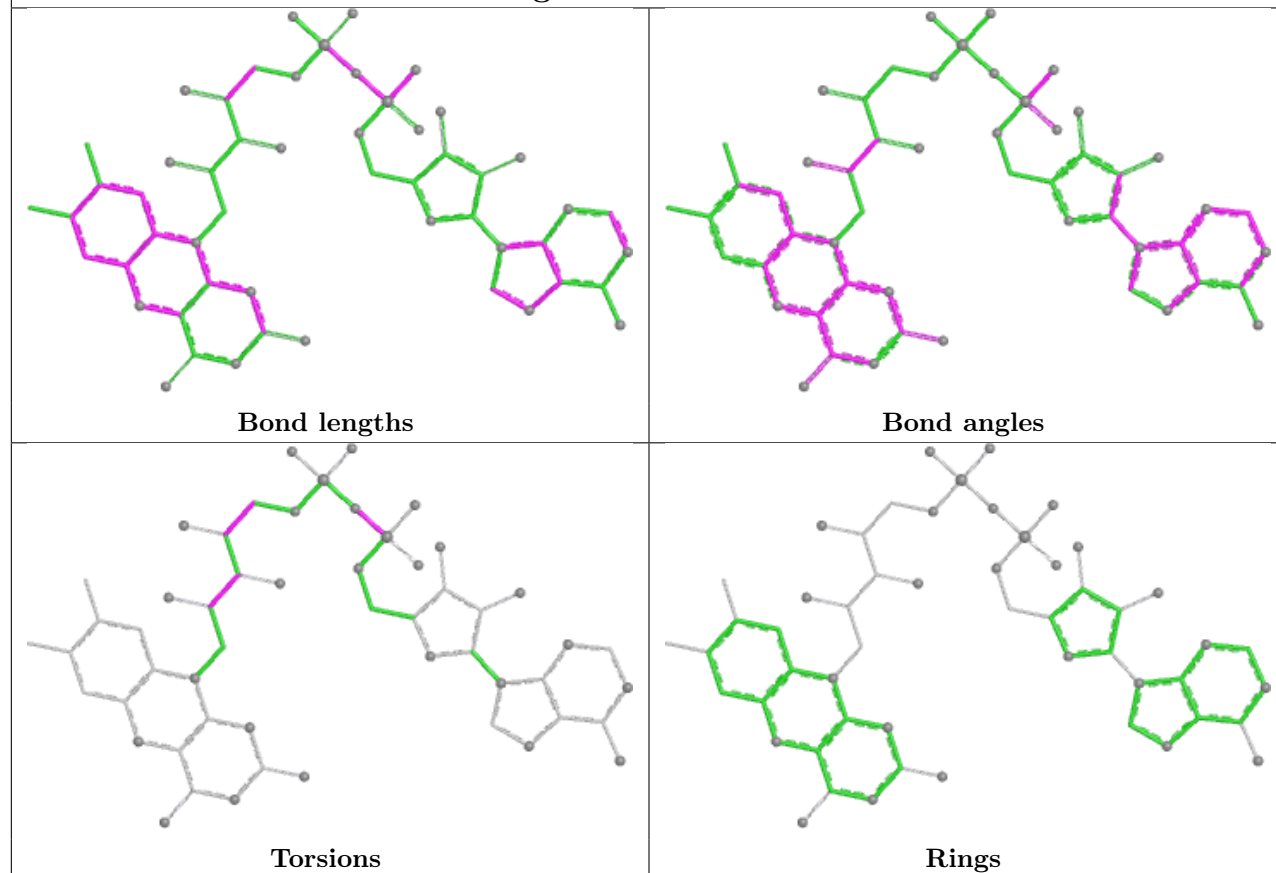
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	FAD	2	0
2	B	301	FAD	2	0
2	A	301	FAD	3	0
3	D	302	MEF	1	0
2	C	301	FAD	1	0

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.

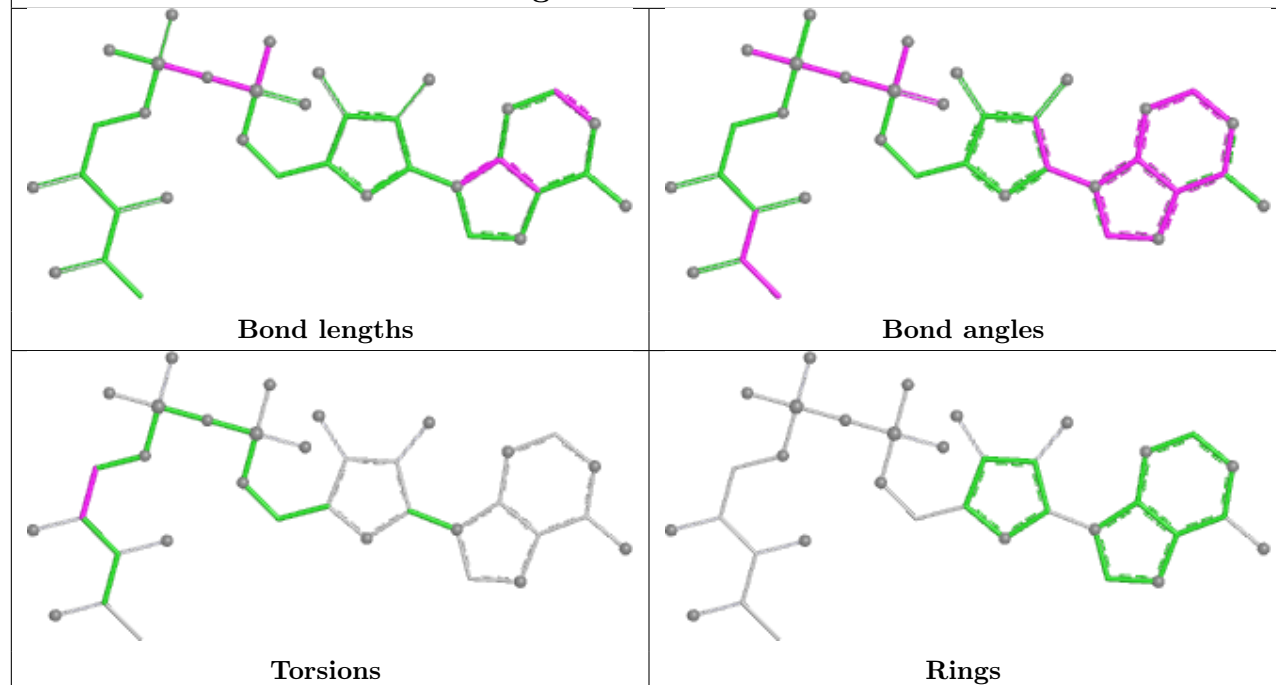


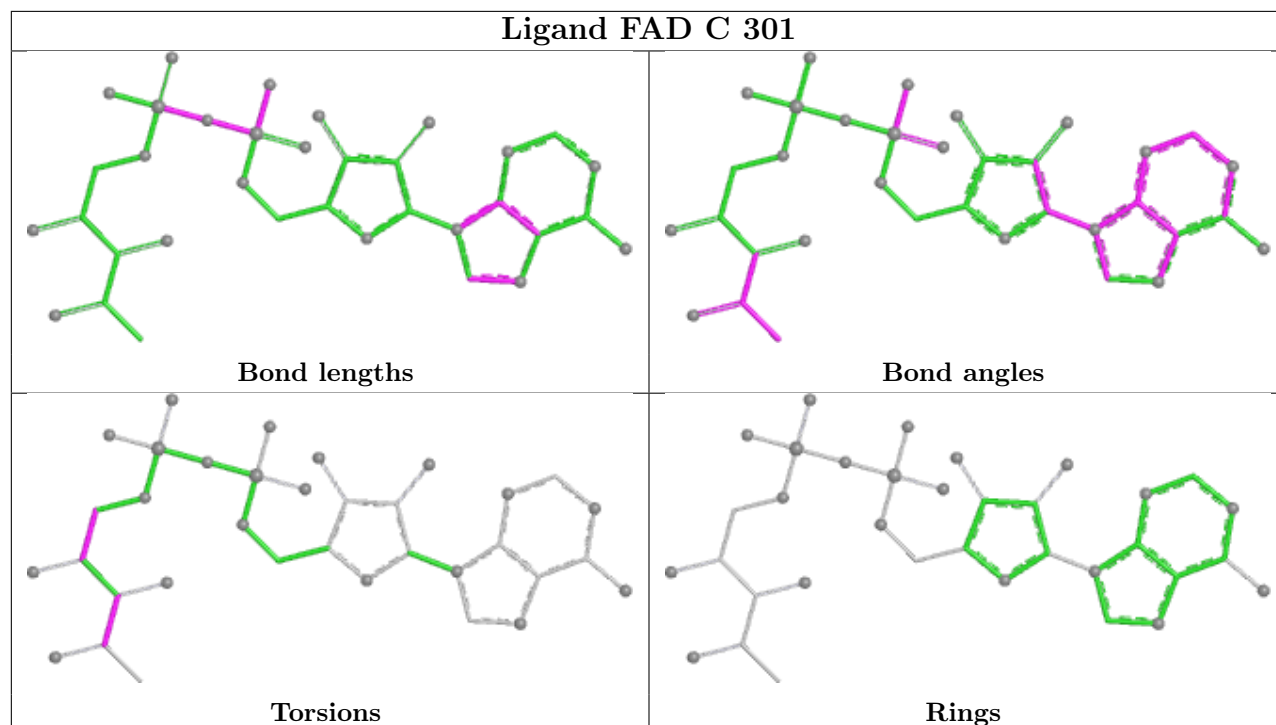
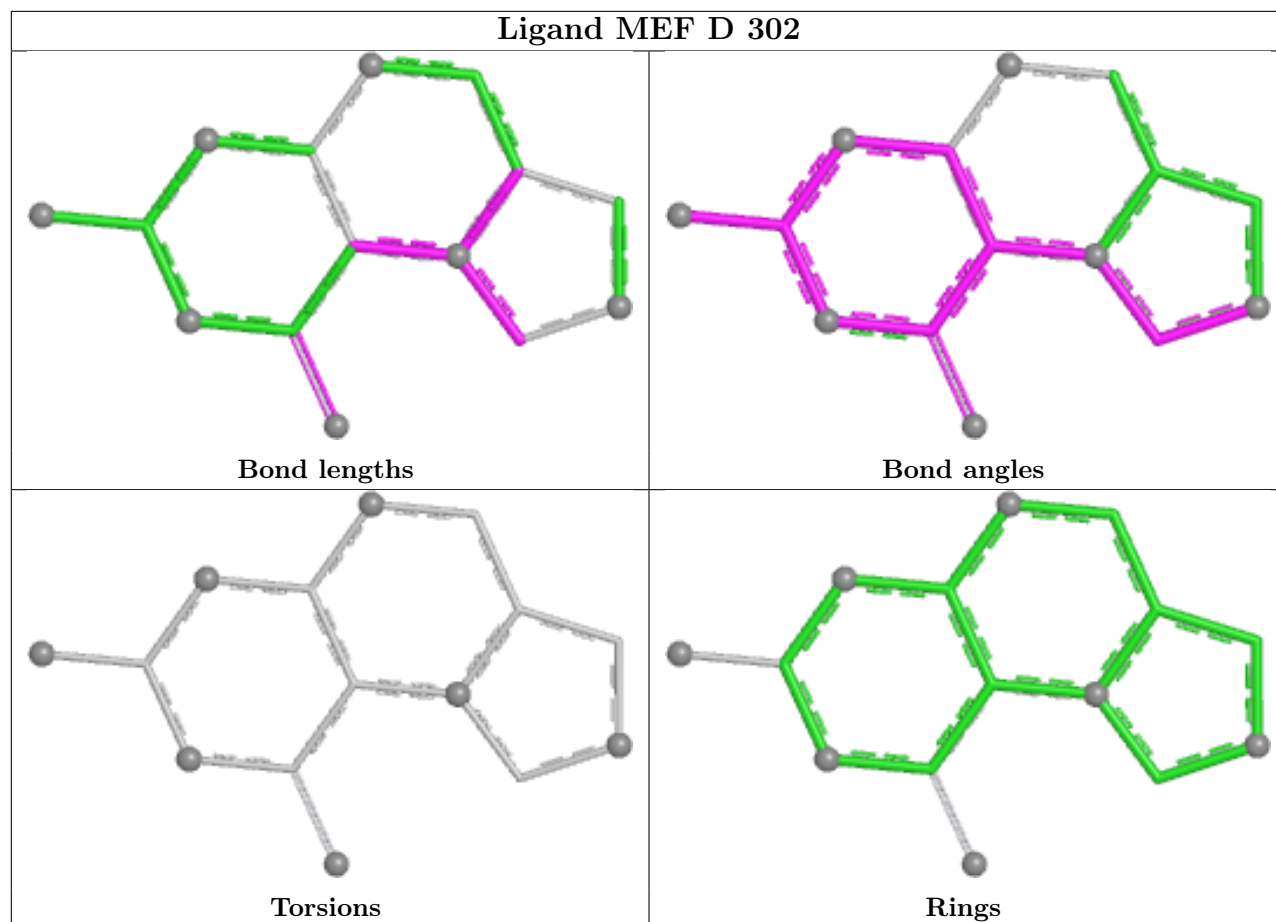


Ligand FAD B 301



Ligand FAD A 301





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	215/232 (92%)	0.28	12 (5%) 30 32	20, 35, 62, 75	1 (0%)
1	B	214/232 (92%)	0.37	11 (5%) 33 36	15, 37, 69, 86	1 (0%)
1	C	217/232 (93%)	0.21	4 (1%) 67 71	22, 35, 61, 79	0
1	D	214/232 (92%)	0.27	10 (4%) 36 39	18, 37, 67, 91	2 (0%)
All	All	860/928 (92%)	0.28	37 (4%) 40 42	15, 36, 65, 91	4 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	SER	4.1
1	A	33	MET	3.8
1	B	89	GLY	3.7
1	B	94	LEU	3.6
1	B	31	PHE	3.5
1	C	31	PHE	3.3
1	B	220	VAL	3.1
1	D	108	GLY	2.9
1	D	32	ASP	2.9
1	A	89	GLY	2.9
1	C	141	VAL	2.8
1	D	110	LYS	2.7
1	B	109	TYR	2.7
1	A	-1	HIS	2.7
1	B	112	THR	2.6
1	C	220	VAL	2.6
1	B	0	HIS	2.6
1	A	31	PHE	2.5
1	B	91	TYR	2.5
1	B	88	SER	2.4
1	C	109	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	139	SER	2.4
1	D	112	THR	2.3
1	A	32	ASP	2.3
1	A	106	LEU	2.2
1	A	107	GLU	2.2
1	A	109	TYR	2.2
1	D	31	PHE	2.2
1	A	112	THR	2.2
1	D	103	PRO	2.2
1	D	138	GLU	2.1
1	B	95	SER	2.1
1	D	113	ILE	2.1
1	B	108	GLY	2.1
1	A	0	HIS	2.1
1	D	53	HIS	2.1
1	D	111	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

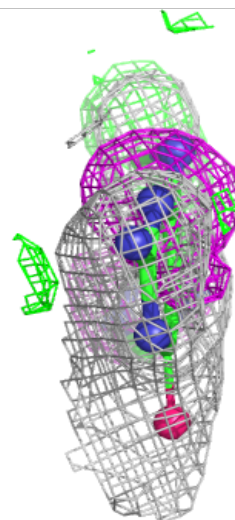
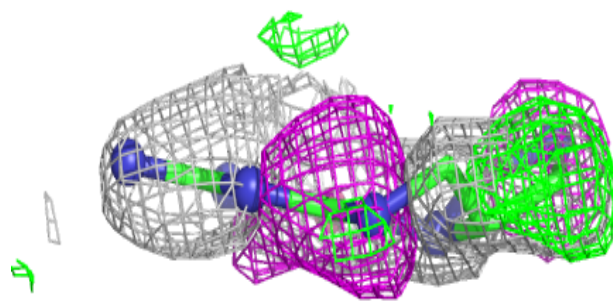
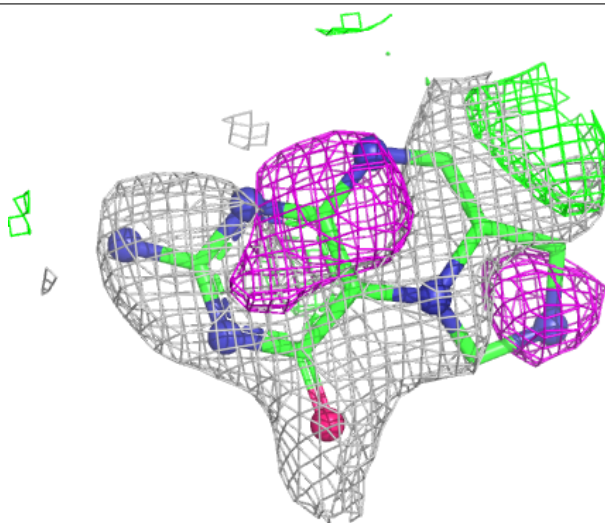
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MEF	B	302	15/33	0.47	0.23	67,73,75,75	0
3	MEF	D	302	15/33	0.54	0.17	51,64,67,67	0
2	FAD	C	301	35/53	0.86	0.13	28,46,55,57	0
2	FAD	B	301	53/53	0.87	0.12	30,48,57,61	0
2	FAD	A	301	35/53	0.87	0.13	30,46,60,65	0
2	FAD	D	301	53/53	0.91	0.10	31,40,49,52	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.

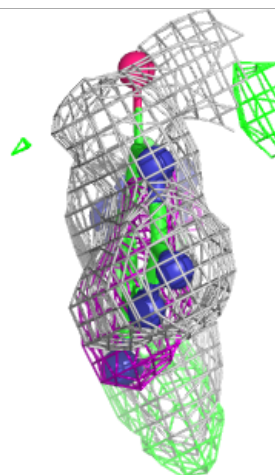
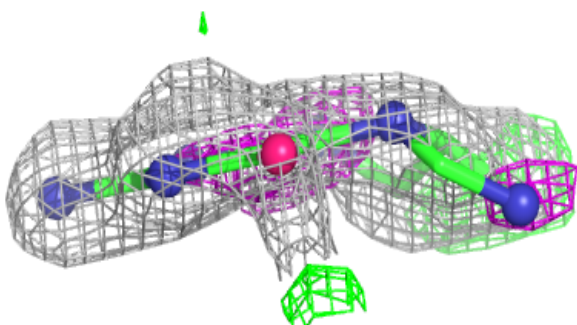
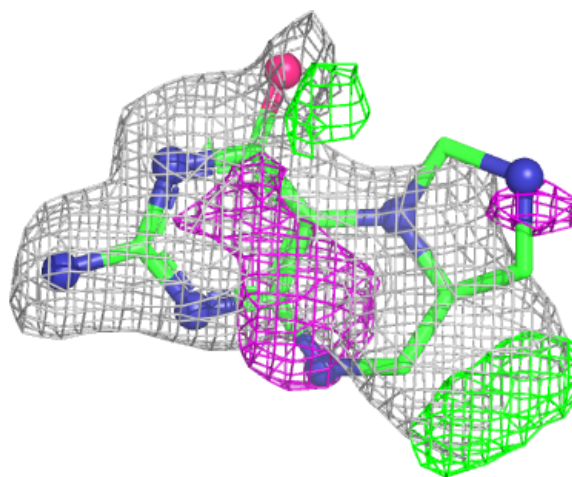
Electron density around MEF B 302:

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



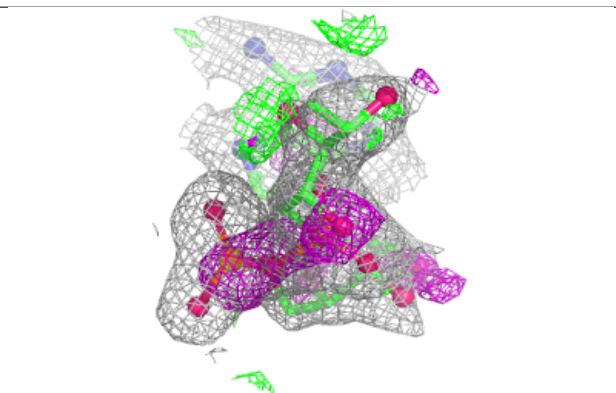
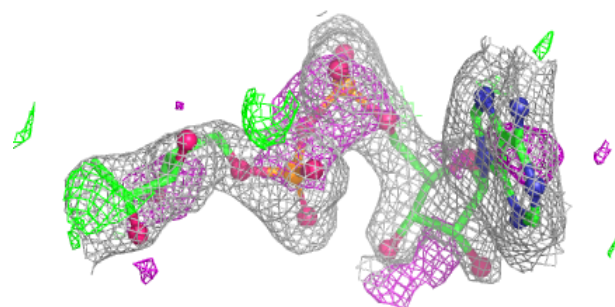
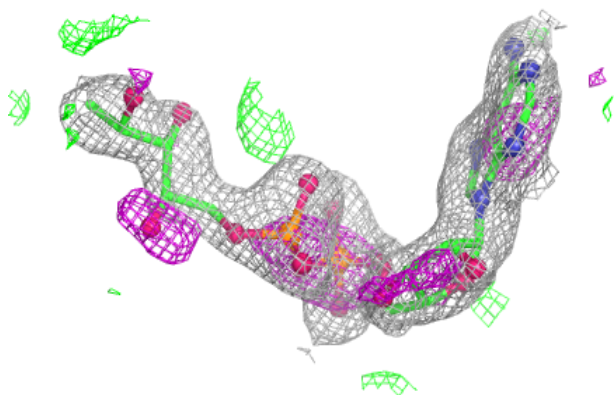
Electron density around MEF D 302:

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

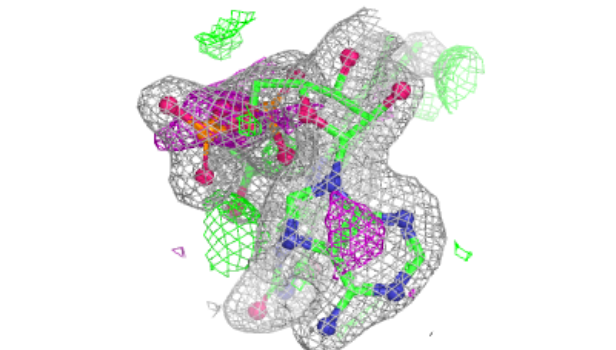
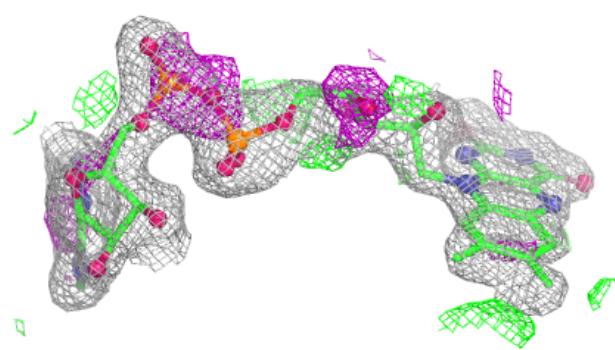
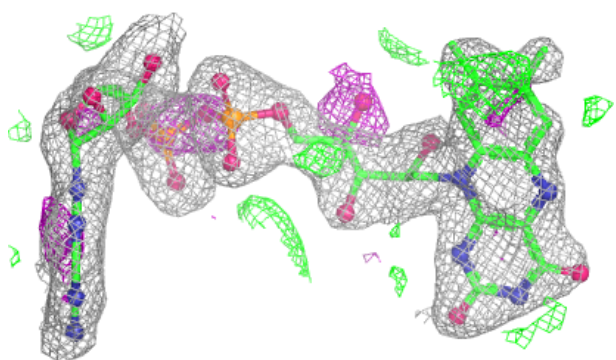


Electron density around FAD C 301:

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

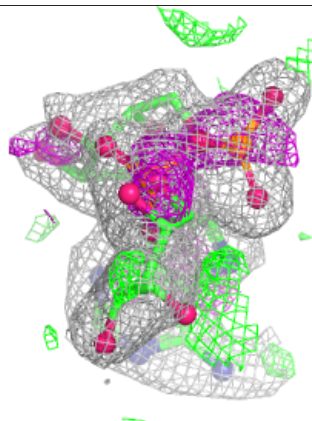
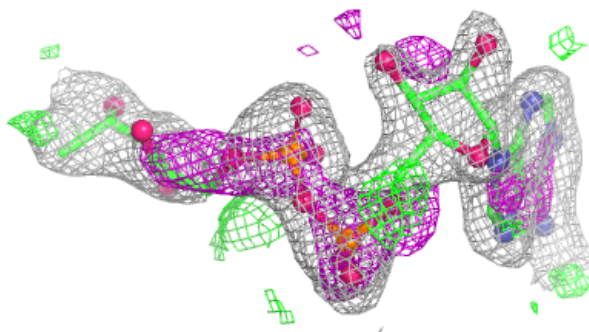
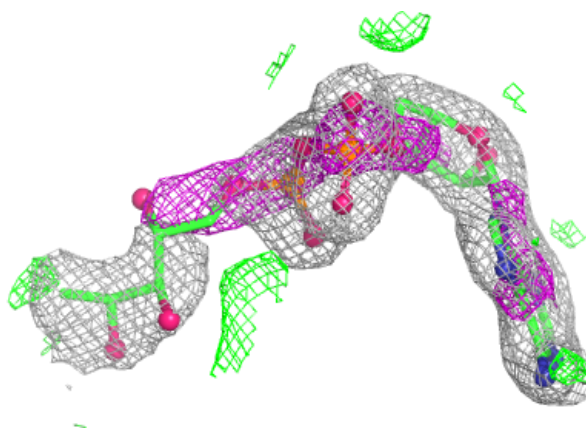
**Electron density around FAD B 301:**

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

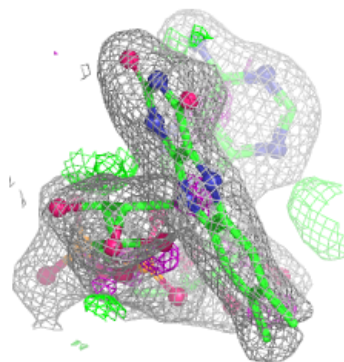
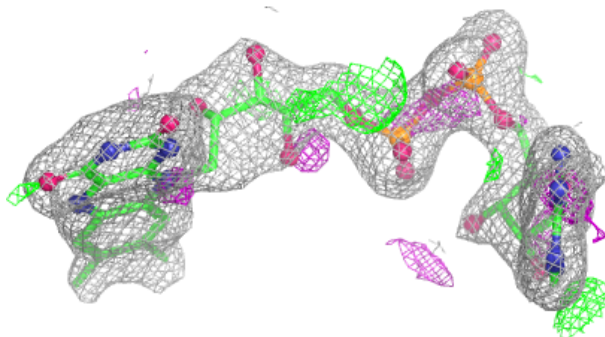
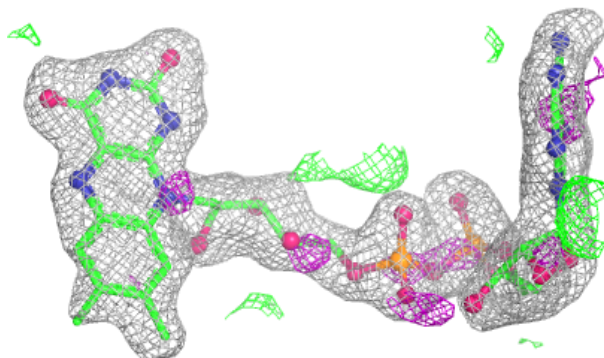


Electron density around FAD A 301:

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

**Electron density around FAD D 301:**

$2mF_o-DF_c$ (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.