



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:21 AM BST

PDB ID : 3G6K
Title : Crystal Structure of Candida glabrata FMN Adenylyltransferase in complex with FAD and Inorganic Pyrophosphate
Authors : Huerta, C.; Machius, M.; Zhang, H.
Deposited on : 2009-02-06
Resolution : 1.35 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 : 2.13
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) : 2.13

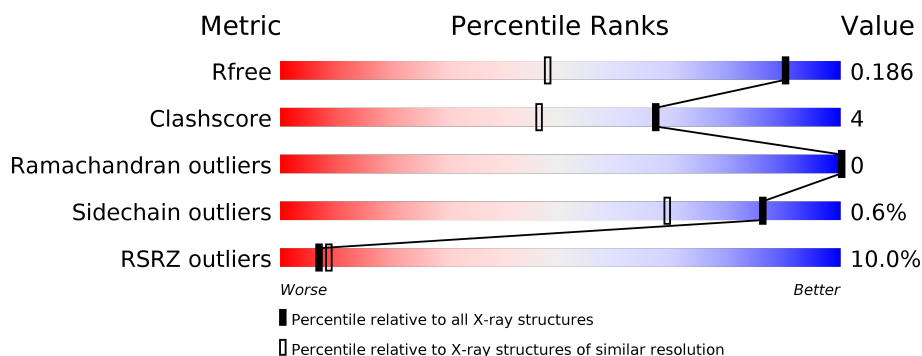
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	308	<div> <div>7%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	B	308	<div> <div>13%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	C	308	<div> <div>8%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	D	308	<div> <div>9%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	E	308	<div> <div>14%</div> <div>86%</div> <div>7%</div> <div>6%</div> </div>
1	F	308	<div> <div>7%</div> <div>92%</div> <div>.</div> <div>.</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17255 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 FMN adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	18	0
			2514	1616	408	481	9			
1	B	305	Total	C	N	O	S	0	17	0
			2576	1659	422	487	8			
1	C	292	Total	C	N	O	S	0	11	0
			2446	1575	400	463	8			
1	D	301	Total	C	N	O	S	0	12	0
			2534	1632	413	482	7			
1	E	288	Total	C	N	O	S	0	13	0
			2419	1561	388	463	7			
1	F	297	Total	C	N	O	S	0	15	0
			2479	1595	403	472	9			

There are 24 discrepancies between the modelled and reference sequences:

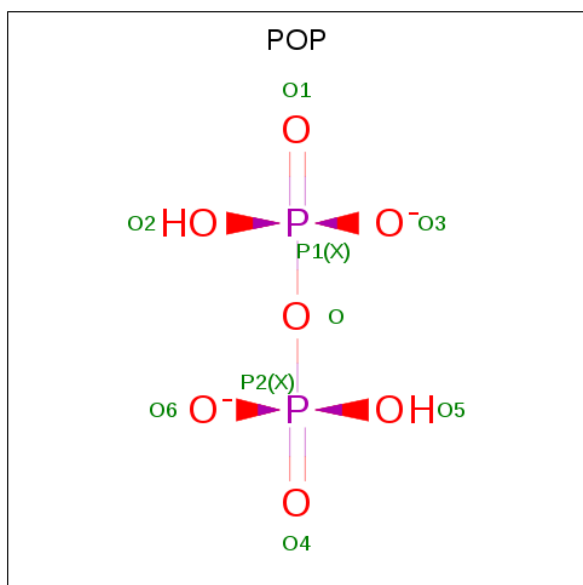
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q6FNA9
A	-2	ALA	-	expression tag	UNP Q6FNA9
A	-1	MET	-	expression tag	UNP Q6FNA9
A	0	VAL	-	expression tag	UNP Q6FNA9
B	-3	GLY	-	expression tag	UNP Q6FNA9
B	-2	ALA	-	expression tag	UNP Q6FNA9
B	-1	MET	-	expression tag	UNP Q6FNA9
B	0	VAL	-	expression tag	UNP Q6FNA9
C	-3	GLY	-	expression tag	UNP Q6FNA9
C	-2	ALA	-	expression tag	UNP Q6FNA9
C	-1	MET	-	expression tag	UNP Q6FNA9
C	0	VAL	-	expression tag	UNP Q6FNA9
D	-3	GLY	-	expression tag	UNP Q6FNA9
D	-2	ALA	-	expression tag	UNP Q6FNA9
D	-1	MET	-	expression tag	UNP Q6FNA9
D	0	VAL	-	expression tag	UNP Q6FNA9
E	-3	GLY	-	expression tag	UNP Q6FNA9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	ALA	-	expression tag	UNP Q6FNA9
E	-1	MET	-	expression tag	UNP Q6FNA9
E	0	VAL	-	expression tag	UNP Q6FNA9
F	-3	GLY	-	expression tag	UNP Q6FNA9
F	-2	ALA	-	expression tag	UNP Q6FNA9
F	-1	MET	-	expression tag	UNP Q6FNA9
F	0	VAL	-	expression tag	UNP Q6FNA9

- Molecule 2 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 9 7 2	0	0
2	B	1	Total O P 9 7 2	0	0
2	C	1	Total O P 9 7 2	0	0
2	D	1	Total O P 9 7 2	0	0
2	E	1	Total O P 9 7 2	0	0
2	F	1	Total O P 9 7 2	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

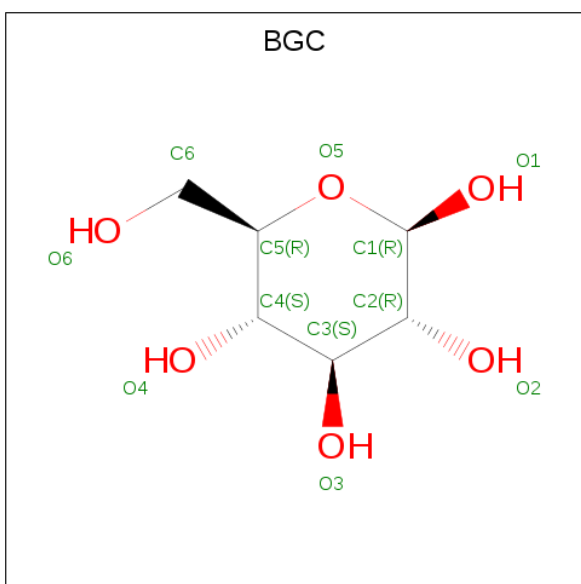
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	B	3	Total	Mg	0	0
			3	3		
4	C	1	Total	Mg	0	0
			1	1		
4	A	3	Total	Mg	0	0
			3	3		
4	F	4	Total	Mg	0	0
			4	4		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			12	6	6		

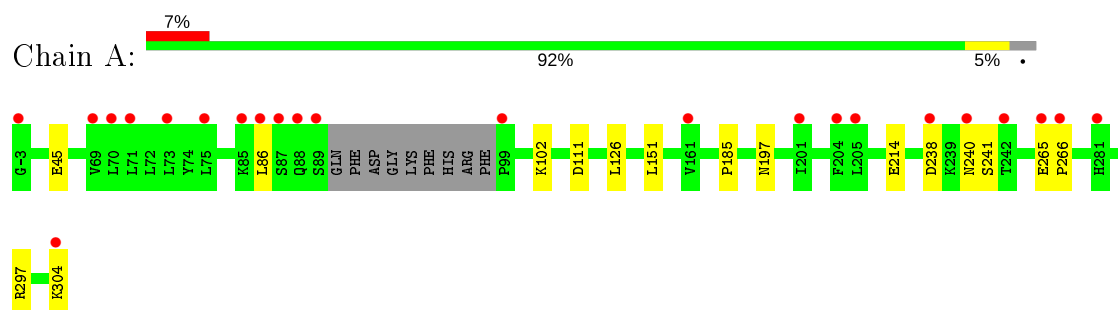
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	343	Total	O	0	0
			343	343		
7	B	308	Total	O	0	0
			308	308		
7	C	309	Total	O	0	0
			309	309		
7	D	326	Total	O	0	0
			326	326		
7	E	239	Total	O	0	0
			239	239		
7	F	345	Total	O	0	0
			345	345		

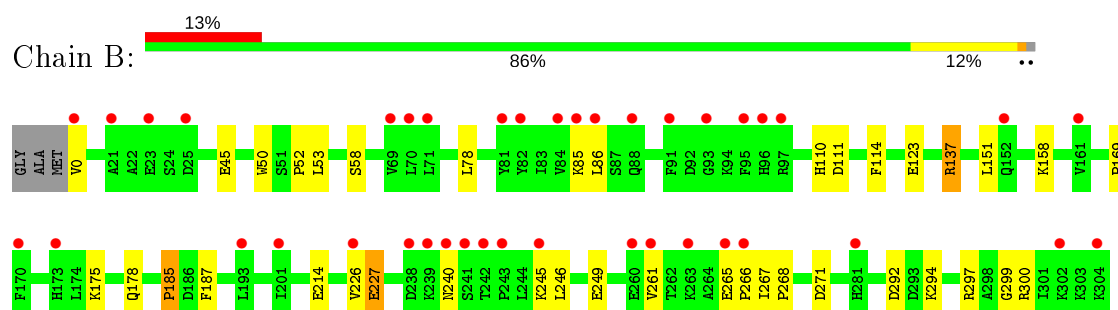
3 Residue-property plots [i](#)

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.

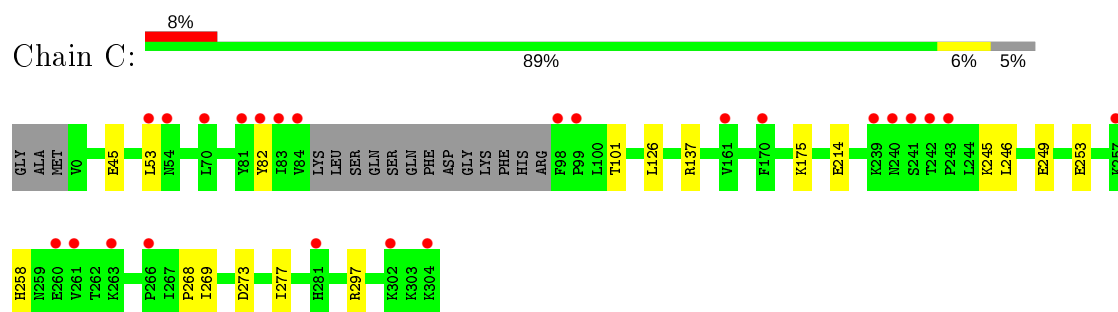
• Molecule 1: FMN adenylyltransferase

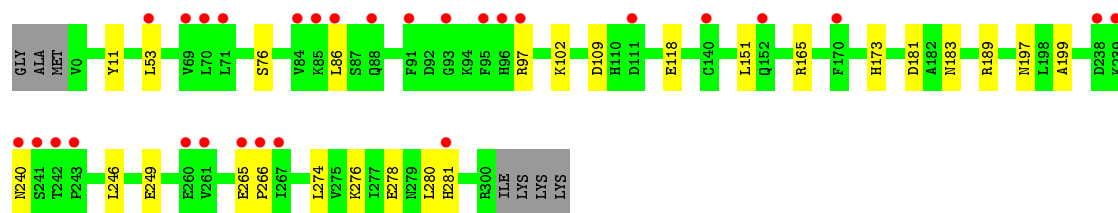


• Molecule 1: FMN adenylyltransferase

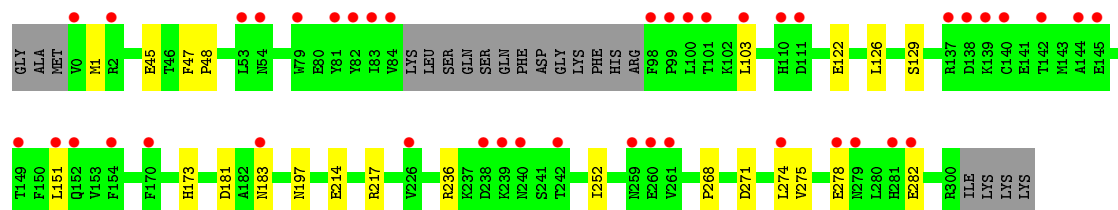
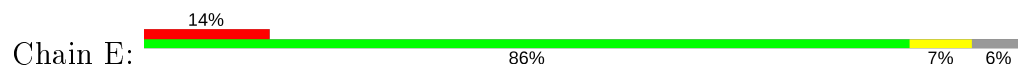


• Molecule 1: FMN adenylyltransferase

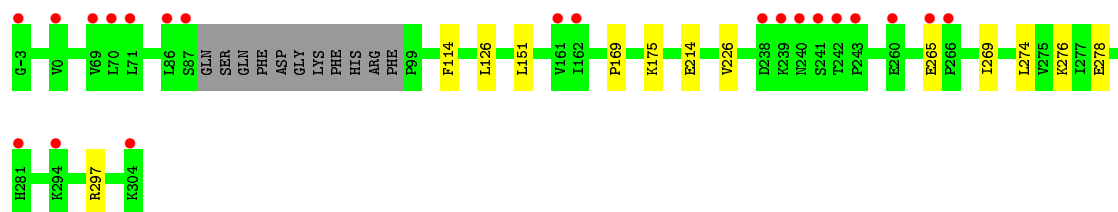




● Molecule 1: FMN adenylyltransferase



● Molecule 1: FMN adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	206.58 Å 81.48 Å 136.60 Å 90.00° 129.79° 90.00°	Depositor
Resolution (Å)	32.19 – 1.35 32.18 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.19-1.35) 99.9 (32.18-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.35 Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.153 , 0.187 0.151 , 0.186	Depositor DCC
R_{free} test set	19043 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17255	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0061e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, BGC, SO4, POP, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.69	0/2666	0.74	1/3620 (0.0%)
1	B	0.70	2/2727 (0.1%)	0.76	6/3701 (0.2%)
1	C	0.67	0/2567	0.74	4/3487 (0.1%)
1	D	0.68	0/2657	0.71	2/3611 (0.1%)
1	E	0.65	0/2546	0.68	1/3467 (0.0%)
1	F	0.74	0/2628	0.76	0/3567
All	All	0.69	2/15791 (0.0%)	0.73	14/21453 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227[A]	GLU	CB-CG	5.41	1.62	1.52
1	B	227[B]	GLU	CB-CG	5.41	1.62	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137[A]	ARG	NE-CZ-NH2	9.17	124.88	120.30
1	B	137[B]	ARG	NE-CZ-NH2	9.17	124.88	120.30
1	B	137[A]	ARG	NE-CZ-NH1	-8.37	116.11	120.30
1	B	137[B]	ARG	NE-CZ-NH1	-8.37	116.11	120.30
1	C	137[A]	ARG	NE-CZ-NH1	-6.78	116.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137[B]	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	B	300[A]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	300[B]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	E	217	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	111	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	165	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	C	137[A]	ARG	CG-CD-NE	-5.12	101.04	111.80
1	C	137[B]	ARG	CG-CD-NE	-5.12	101.04	111.80
1	D	189	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	240	ASN	Peptide

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	2514	0	2465	18	0
1	B	2576	0	2503	47	0
1	C	2446	0	2380	17	0
1	D	2534	0	2451	18	0
1	E	2419	0	2349	19	0
1	F	2479	0	2415	9	0
2	A	9	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
2	D	9	0	0	0	0
2	E	9	0	0	0	0
2	F	9	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
3	C	53	0	31	0	0
3	D	53	0	31	0	0
3	E	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	53	0	31	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	4	0	0	0	0
5	B	5	0	0	0	0
5	D	10	0	0	0	0
5	F	5	0	0	0	0
6	B	12	0	12	0	0
7	A	343	0	0	7	0
7	B	308	0	0	23	0
7	C	309	0	0	9	0
7	D	326	0	0	3	0
7	E	239	0	0	7	0
7	F	345	0	0	2	0
All	All	17255	0	14761	118	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 4.

All (118) 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:C:214[A]:GLU:OE2	7:C:1853:HOH:O	1.57	1.20
1:A:197[B]:ASN:ND2	7:A:1822:HOH:O	1.70	1.19
1:E:214:GLU:OE2	7:E:1716:HOH:O	1.65	1.10
1:E:197[B]:ASN:ND2	7:E:1278:HOH:O	1.85	1.07
1:B:227[A]:GLU:HG2	1:D:197[A]:ASN:ND2	1.77	1.00
1:E:45:GLU:OE2	7:E:753:HOH:O	1.86	0.93
1:B:227[A]:GLU:OE1	7:B:1079:HOH:O	1.89	0.89
1:A:238[A]:ASP:OD2	1:A:241:SER:OG	1.92	0.87
1:B:175[A]:LYS:CD	7:B:1221:HOH:O	2.26	0.82
1:B:45:GLU:OE2	7:B:1076:HOH:O	1.98	0.81
1:A:297[A]:ARG:NE	7:A:1823:HOH:O	1.74	0.81
1:B:58[A]:SER:OG	7:B:1388:HOH:O	1.98	0.81
1:C:214[B]:GLU:OE2	7:C:948:HOH:O	1.99	0.79
1:D:276:LYS:HD3	7:D:1588:HOH:O	1.84	0.79
1:A:297[A]:ARG:CZ	7:A:1823:HOH:O	2.27	0.74
1:D:265:GLU:HB2	1:D:266:PRO:HD2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297[A]:ARG:NH1	7:A:1823:HOH:O	2.21	0.74
1:B:271:ASP:HB3	7:B:816:HOH:O	1.86	0.73
1:E:181[B]:ASP:OD1	1:E:183:ASN:OD1	2.08	0.71
1:B:175[A]:LYS:HD3	7:B:1221:HOH:O	1.89	0.71
1:F:214[B]:GLU:OE2	7:F:1507:HOH:O	2.10	0.69
1:B:271:ASP:OD2	7:B:1709:HOH:O	2.09	0.69
1:B:214[B]:GLU:OE1	7:B:1298:HOH:O	2.09	0.69
1:B:175[A]:LYS:HD2	7:B:1396:HOH:O	1.92	0.68
1:A:126[B]:LEU:HD21	1:F:126[B]:LEU:HD21	1.74	0.68
1:B:0:VAL:HB	7:E:1328:HOH:O	1.94	0.68
1:C:253:GLU:HG3	7:C:1632:HOH:O	1.94	0.67
7:B:1249:HOH:O	1:E:126:LEU:HD21	1.93	0.67
7:B:1249:HOH:O	1:E:126:LEU:CD2	2.43	0.66
1:B:114:PHE:HA	1:B:226[B]:VAL:CG1	2.26	0.65
1:C:45:GLU:OE1	7:C:401:HOH:O	2.14	0.64
1:B:245:LYS:HG2	7:B:857:HOH:O	1.98	0.61
1:A:304:LYS:HD3	1:C:245:LYS:HB3	1.83	0.61
1:D:109:ASP:OD1	1:D:118[B]:GLU:OE2	2.19	0.60
1:B:271:ASP:OD1	1:E:271:ASP:OD2	2.19	0.59
1:A:238[A]:ASP:CG	1:A:241:SER:OG	2.39	0.59
1:D:181[B]:ASP:OD1	1:D:183:ASN:OD1	2.21	0.59
1:B:246:LEU:HD23	1:B:249:GLU:HG2	1.85	0.58
1:D:265:GLU:CB	1:D:266:PRO:HD2	2.34	0.58
1:C:273:ASP:O	1:C:277:ILE:HD12	2.04	0.57
1:E:268:PRO:HD2	7:E:1134:HOH:O	2.04	0.57
1:B:111:ASP:HA	1:B:137[B]:ARG:HG3	1.87	0.57
1:B:50:TRP:CD1	1:B:158:LYS:HE2	2.39	0.57
1:A:238[B]:ASP:OD1	1:A:240:ASN:OD1	2.23	0.57
1:D:280:LEU:O	1:D:281:HIS:HB2	2.04	0.56
1:E:173[B]:HIS:HE1	7:E:1272:HOH:O	1.89	0.56
1:C:297[B]:ARG:NH1	7:C:641:HOH:O	2.31	0.56
1:A:45:GLU:OE2	7:A:555:HOH:O	2.18	0.55
1:B:85:LYS:HE2	7:B:1414:HOH:O	2.08	0.54
1:D:173[B]:HIS:HB3	1:E:268:PRO:HG3	1.90	0.54
1:B:151:LEU:HD12	1:B:185:PRO:HB2	1.89	0.54
1:D:102:LYS:HE3	7:D:391:HOH:O	2.09	0.53
1:F:114:PHE:HA	1:F:226[B]:VAL:CG1	2.38	0.53
1:B:52:PRO:HB2	1:B:78[B]:LEU:HD21	1.88	0.53
1:B:137[B]:ARG:NH2	7:B:1820:HOH:O	2.25	0.52
1:B:292:ASP:OD1	1:B:294:LYS:HG2	2.09	0.52
1:C:175:LYS:HE3	1:F:269:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ASN:HB3	7:D:774:HOH:O	2.10	0.51
1:E:1:MET:O	1:E:129:SER:OG	2.23	0.51
1:B:227[A]:GLU:HG2	1:D:197[A]:ASN:CG	2.29	0.50
1:D:183:ASN:HA	1:E:252:ILE:CG2	2.42	0.49
1:D:265:GLU:HB2	1:D:266:PRO:CD	2.41	0.49
1:B:123:GLU:OE2	1:E:122:GLU:OE1	2.30	0.49
1:A:214[A]:GLU:OE1	7:A:1622:HOH:O	2.20	0.48
1:B:110:HIS:C	1:B:137[B]:ARG:HG3	2.33	0.48
1:E:274:LEU:HD11	1:E:278:GLU:OE2	2.14	0.47
1:D:11:TYR:HA	1:D:76[B]:SER:HB2	1.96	0.47
1:B:265:GLU:HG3	1:B:266:PRO:HD2	1.96	0.47
1:A:151:LEU:CD1	1:A:185:PRO:HB2	2.45	0.47
1:B:297[A]:ARG:NE	7:B:1870:HOH:O	2.26	0.47
1:B:137[B]:ARG:NE	7:B:1820:HOH:O	2.35	0.46
1:B:178:GLN:HB3	7:B:1396:HOH:O	2.14	0.46
1:A:238[A]:ASP:OD1	1:A:241:SER:OG	2.33	0.46
1:B:52:PRO:HB2	1:B:78[B]:LEU:CD2	2.45	0.46
1:C:249:GLU:O	1:C:253:GLU:HG3	2.16	0.46
7:B:1079:HOH:O	1:D:199:ALA:HB3	2.15	0.46
1:F:276:LYS:HE2	1:F:276:LYS:HB2	1.71	0.46
1:C:269:ILE:HD11	1:C:277:ILE:HD13	1.98	0.45
1:B:158:LYS:HE3	7:B:348:HOH:O	2.16	0.45
1:A:151:LEU:HD12	1:A:185:PRO:HB2	1.99	0.44
1:F:169:PRO:HD3	1:F:297[B]:ARG:NH1	2.32	0.44
1:B:53:LEU:HD11	1:B:86:LEU:HD11	1.99	0.44
1:D:53:LEU:HD11	1:D:86:LEU:HD11	1.99	0.44
1:C:258[B]:HIS:HD2	7:C:1676:HOH:O	2.00	0.44
1:B:245:LYS:HE3	7:B:1784:HOH:O	2.18	0.44
1:C:297[B]:ARG:NH2	7:C:1824:HOH:O	2.45	0.43
1:D:274:LEU:HD11	1:D:278:GLU:OE2	2.19	0.43
1:F:175:LYS:NZ	7:F:440:HOH:O	2.47	0.43
1:B:151:LEU:HD11	1:B:187:PHE:CD1	2.54	0.43
1:B:175[A]:LYS:HE3	7:B:1221:HOH:O	2.19	0.43
1:C:126:LEU:HD21	7:C:1098:HOH:O	2.19	0.42
1:B:114:PHE:CD1	1:B:226[B]:VAL:HG12	2.55	0.42
1:B:111:ASP:HA	1:B:137[B]:ARG:CG	2.48	0.42
1:A:102:LYS:NZ	7:A:1522:HOH:O	2.52	0.41
1:C:214[A]:GLU:CD	1:C:268:PRO:HA	2.40	0.41
1:B:114:PHE:HA	1:B:226[B]:VAL:HG12	2.01	0.41
1:B:267:ILE:HA	1:B:268:PRO:HD3	1.80	0.41
1:F:274:LEU:HD11	1:F:278:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LEU:HD11	1:B:187:PHE:HD1	1.85	0.41
1:B:169:PRO:HD3	1:B:297[B]:ARG:NH2	2.35	0.41
1:E:275:VAL:HG13	7:E:1830:HOH:O	2.20	0.41
1:C:53:LEU:HD21	1:C:82:TYR:CE2	2.56	0.41
1:B:151:LEU:HD12	1:B:185:PRO:CB	2.50	0.41
1:C:101:THR:CG2	7:C:443:HOH:O	2.69	0.41
1:B:261:VAL:HG13	7:B:1611:HOH:O	2.21	0.40
1:D:246:LEU:HD23	1:D:249[A]:GLU:HG2	2.02	0.40
1:A:151:LEU:HD12	1:A:185:PRO:CB	2.51	0.40
1:B:151:LEU:CD1	1:B:185:PRO:HB2	2.50	0.40
1:F:114:PHE:HA	1:F:226[B]:VAL:HG12	2.03	0.40
1:A:265:GLU:HG3	1:A:266:PRO:HD2	2.02	0.40
1:A:304:LYS:HD2	1:C:246:LEU:O	2.21	0.40
1:B:297[A]:ARG:NH1	7:B:1870:HOH:O	2.44	0.40
1:E:47:PHE:N	1:E:48:PRO:CD	2.85	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	313/308 (102%)	311 (99%)	2 (1%)	0	100	100
1	B	320/308 (104%)	316 (99%)	4 (1%)	0	100	100
1	C	299/308 (97%)	296 (99%)	3 (1%)	0	100	100
1	D	311/308 (101%)	309 (99%)	2 (1%)	0	100	100
1	E	297/308 (96%)	294 (99%)	3 (1%)	0	100	100
1	F	308/308 (100%)	305 (99%)	3 (1%)	0	100	100
All	All	1848/1848 (100%)	1831 (99%)	17 (1%)	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	291/281 (104%)	290 (100%)	1 (0%)	92	83
1	B	295/281 (105%)	293 (99%)	2 (1%)	84	64
1	C	279/281 (99%)	279 (100%)	0	100	100
1	D	288/281 (102%)	286 (99%)	2 (1%)	84	64
1	E	277/281 (99%)	274 (99%)	3 (1%)	73	45
1	F	286/281 (102%)	284 (99%)	2 (1%)	84	64
All	All	1716/1686 (102%)	1706 (99%)	10 (1%)	86	69

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	B	185	PRO
1	B	240	ASN
1	D	97	ARG
1	D	151	LEU
1	E	151	LEU
1	E	282[A]	GLU
1	E	282[B]	GLU
1	F	151	LEU
1	F	265	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	62	ASN
1	E	62	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 13 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	B	310	-	4,4,4	0.18	0	6,6,6	0.32	0
2	POP	A	305	4	6,8,8	1.30	0	13,13,13	0.98	1 (7%)
2	POP	C	305	4	6,8,8	0.92	0	13,13,13	0.78	0
5	SO4	D	309	-	4,4,4	0.22	0	6,6,6	0.27	0
2	POP	B	305	4	6,8,8	0.82	0	13,13,13	0.71	0
2	POP	F	305	4	6,8,8	1.23	1 (16%)	13,13,13	1.00	1 (7%)
3	FAD	E	306	4	51,58,58	1.49	6 (11%)	60,89,89	1.76	7 (11%)
3	FAD	C	306	4	51,58,58	1.28	7 (13%)	60,89,89	1.57	8 (13%)
3	FAD	A	306	4	51,58,58	1.50	8 (15%)	60,89,89	1.77	8 (13%)
6	BGC	B	311	-	12,12,12	0.51	0	17,17,17	1.37	3 (17%)
3	FAD	F	306	4	51,58,58	1.32	6 (11%)	60,89,89	1.49	5 (8%)
3	FAD	D	306	4	51,58,58	1.37	8 (15%)	60,89,89	1.45	9 (15%)
3	FAD	B	306	4	51,58,58	1.55	8 (15%)	60,89,89	1.72	8 (13%)
5	SO4	F	311	-	4,4,4	0.26	0	6,6,6	0.72	0
2	POP	E	305	4	6,8,8	0.79	0	13,13,13	0.95	0
5	SO4	D	308	-	4,4,4	0.12	0	6,6,6	0.46	0
2	POP	D	305	4	6,8,8	0.94	0	13,13,13	0.85	0

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	POP	A	305	4	-	0/6/6/6	-
2	POP	F	305	4	-	0/6/6/6	-
2	POP	C	305	4	-	0/6/6/6	-
2	POP	B	305	4	-	0/6/6/6	-
3	FAD	E	306	4	-	0/30/50/50	0/6/6/6
3	FAD	C	306	4	-	1/30/50/50	0/6/6/6
3	FAD	A	306	4	-	1/30/50/50	0/6/6/6
6	BGC	B	311	-	-	2/2/22/22	0/1/1/1
3	FAD	F	306	4	-	0/30/50/50	0/6/6/6
3	FAD	D	306	4	-	0/30/50/50	0/6/6/6
3	FAD	B	306	4	-	0/30/50/50	0/6/6/6
2	POP	E	305	4	-	0/6/6/6	-
2	POP	D	305	4	-	0/6/6/6	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	306	FAD	C2A-N3A	4.92	1.40	1.32
3	C	306	FAD	C4X-N5	4.81	1.40	1.33
3	B	306	FAD	C2A-N3A	4.72	1.39	1.32
3	E	306	FAD	C4-N3	4.45	1.40	1.33
3	B	306	FAD	C10-N1	4.44	1.39	1.33
3	E	306	FAD	C4X-N5	4.09	1.39	1.33
3	B	306	FAD	C5X-N5	4.08	1.42	1.35
3	A	306	FAD	C4X-N5	4.02	1.39	1.33
3	D	306	FAD	C2A-N3A	4.02	1.38	1.32
3	A	306	FAD	C5X-N5	3.90	1.41	1.35
3	B	306	FAD	C4X-N5	3.69	1.38	1.33
3	D	306	FAD	C1'-N10	3.53	1.51	1.48
3	A	306	FAD	P-O1P	-3.52	1.38	1.50
3	F	306	FAD	C2A-N3A	3.35	1.37	1.32
3	C	306	FAD	C2A-N3A	3.34	1.37	1.32
3	D	306	FAD	C4X-N5	3.33	1.38	1.33
3	A	306	FAD	C1'-N10	3.24	1.51	1.48
3	F	306	FAD	C4-N3	3.18	1.38	1.33
3	F	306	FAD	C4X-N5	3.17	1.37	1.33
3	E	306	FAD	C1'-N10	3.11	1.51	1.48
3	A	306	FAD	C4-N3	3.06	1.38	1.33
3	F	306	FAD	C5X-N5	3.03	1.40	1.35
3	A	306	FAD	C10-N1	3.00	1.37	1.33
3	E	306	FAD	C5X-N5	2.97	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	306	FAD	C1'-N10	2.86	1.51	1.48
3	C	306	FAD	C10-N1	2.73	1.36	1.33
3	D	306	FAD	C4-N3	2.61	1.37	1.33
3	A	306	FAD	O4B-C1B	2.61	1.44	1.41
3	A	306	FAD	C2A-N3A	2.59	1.36	1.32
3	E	306	FAD	C10-N1	2.59	1.36	1.33
3	F	306	FAD	C6-C5X	-2.48	1.38	1.41
3	B	306	FAD	C4-N3	2.39	1.37	1.33
3	F	306	FAD	O4B-C1B	2.33	1.44	1.41
3	B	306	FAD	C9A-C5X	-2.24	1.38	1.42
3	D	306	FAD	C6-C5X	-2.21	1.38	1.41
3	D	306	FAD	C10-N1	2.20	1.36	1.33
3	C	306	FAD	C5X-N5	2.17	1.38	1.35
3	D	306	FAD	C4X-C10	2.15	1.41	1.38
3	C	306	FAD	P-O1P	-2.11	1.43	1.50
3	B	306	FAD	C2A-N1A	2.10	1.37	1.33
3	C	306	FAD	C6-C5X	-2.09	1.38	1.41
3	D	306	FAD	C5X-N5	2.05	1.38	1.35
3	C	306	FAD	O4B-C1B	2.04	1.43	1.41
2	F	305	POP	P2-O6	-2.01	1.47	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	306	FAD	C4-N3-C2	8.14	122.01	115.14
3	B	306	FAD	C4-N3-C2	7.38	121.37	115.14
3	E	306	FAD	N3A-C2A-N1A	-7.12	117.54	128.68
3	F	306	FAD	C4-N3-C2	6.75	120.84	115.14
3	C	306	FAD	C4-N3-C2	6.61	120.72	115.14
3	D	306	FAD	C4-N3-C2	6.59	120.71	115.14
3	E	306	FAD	C1'-N10-C9A	6.30	123.25	118.29
3	C	306	FAD	N3A-C2A-N1A	-5.40	120.24	128.68
3	E	306	FAD	C4-N3-C2	5.29	119.61	115.14
3	A	306	FAD	C5X-C9A-N10	4.92	121.28	117.72
3	B	306	FAD	N3A-C2A-N1A	-4.77	121.22	128.68
3	F	306	FAD	N3A-C2A-N1A	-4.48	121.68	128.68
3	A	306	FAD	C4X-C4-N3	-3.77	118.28	123.43
3	A	306	FAD	N3A-C2A-N1A	-3.59	123.07	128.68
3	B	306	FAD	C4X-N5-C5X	3.57	120.34	116.77
3	F	306	FAD	C4X-C4-N3	-3.48	118.67	123.43
3	C	306	FAD	C1'-N10-C9A	3.23	120.84	118.29
3	B	306	FAD	C5X-C9A-N10	3.22	120.05	117.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	306	FAD	C4X-C4-N3	-3.22	119.03	123.43
3	F	306	FAD	C1'-N10-C10	3.11	121.19	118.41
3	D	306	FAD	N3A-C2A-N1A	-3.05	123.90	128.68
3	A	306	FAD	C1'-N10-C10	3.03	121.12	118.41
6	B	311	BGC	C1-C2-C3	2.99	116.52	110.31
3	D	306	FAD	C1'-N10-C9A	2.95	120.62	118.29
3	C	306	FAD	C4X-C4-N3	-2.93	119.43	123.43
3	E	306	FAD	C4X-C4-N3	-2.69	119.75	123.43
3	B	306	FAD	C4X-C4-N3	-2.62	119.84	123.43
3	B	306	FAD	C9A-C5X-N5	-2.60	118.29	122.36
3	B	306	FAD	C1B-N9A-C4A	-2.50	122.25	126.64
3	E	306	FAD	C2A-N1A-C6A	2.50	123.03	118.75
3	D	306	FAD	C4A-C5A-N7A	-2.41	106.89	109.40
3	B	306	FAD	C4X-C10-N10	-2.34	117.90	120.30
3	E	306	FAD	O2A-PA-O5B	2.32	118.53	107.75
3	F	306	FAD	C5X-C9A-N10	2.31	119.39	117.72
3	A	306	FAD	O5'-P-O1P	-2.27	100.18	109.07
3	D	306	FAD	C4-C4X-N5	2.25	121.17	118.60
3	C	306	FAD	C2A-N1A-C6A	2.25	122.60	118.75
3	A	306	FAD	C9A-N10-C10	-2.22	119.00	121.91
6	B	311	BGC	O3-C3-C2	-2.21	105.24	110.35
3	A	306	FAD	C4A-C5A-N7A	-2.19	107.12	109.40
6	B	311	BGC	O5-C1-C2	2.17	114.15	110.28
3	C	306	FAD	C4X-N5-C5X	2.16	118.94	116.77
3	C	306	FAD	O5'-P-O1P	-2.12	100.80	109.07
3	E	306	FAD	C4-C4X-C10	-2.11	118.55	119.95
3	D	306	FAD	C4'-C3'-C2'	-2.11	108.97	113.36
2	A	305	POP	O6-P2-O5	2.08	115.60	107.64
3	D	306	FAD	C4-C4X-C10	-2.07	118.58	119.95
2	F	305	POP	O6-P2-O5	2.06	115.50	107.64
3	C	306	FAD	C10-C4X-N5	-2.04	119.85	121.26
3	D	306	FAD	P-O3P-PA	-2.00	125.96	132.83

There are no chirality outliers.

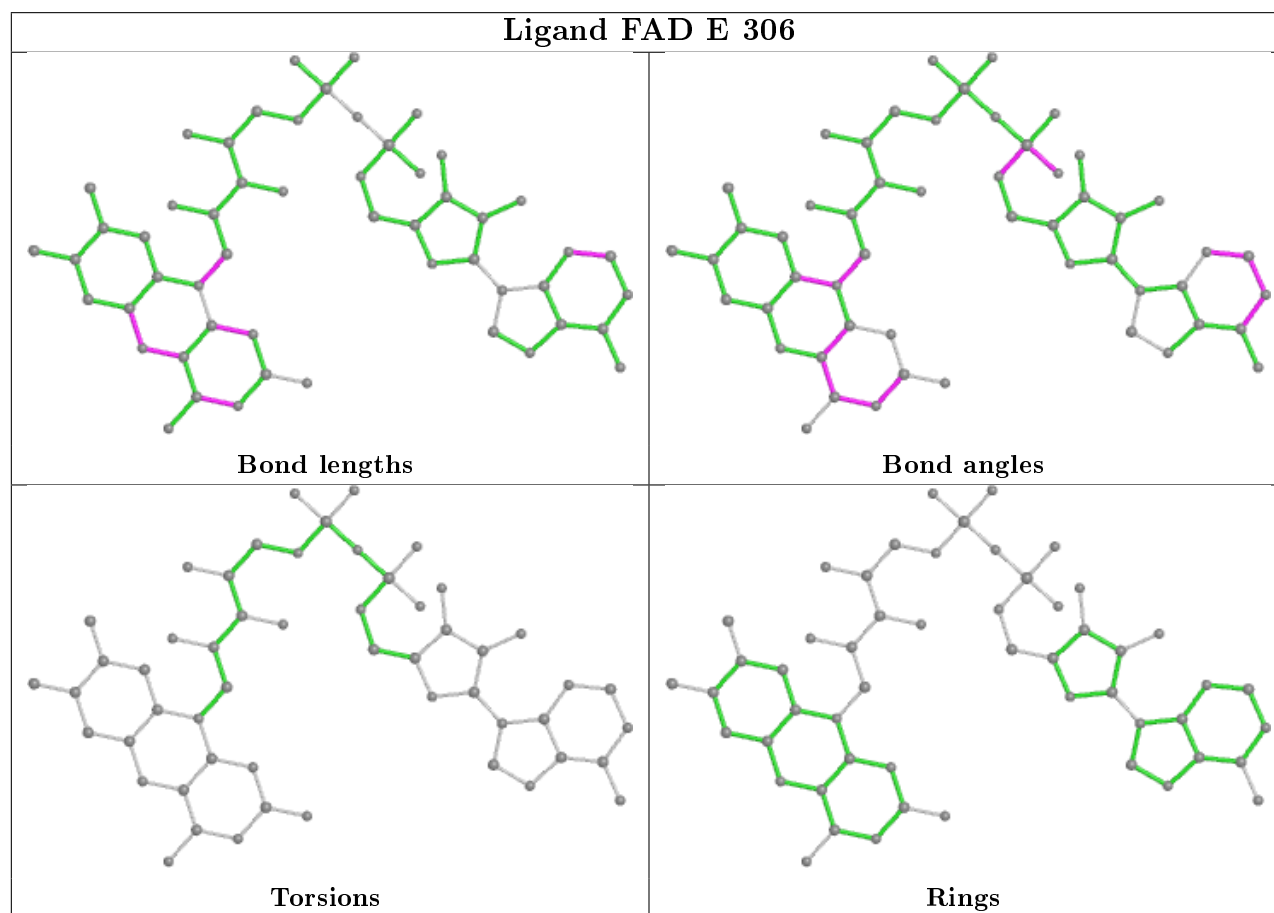
All (4) torsion outliers are listed below:

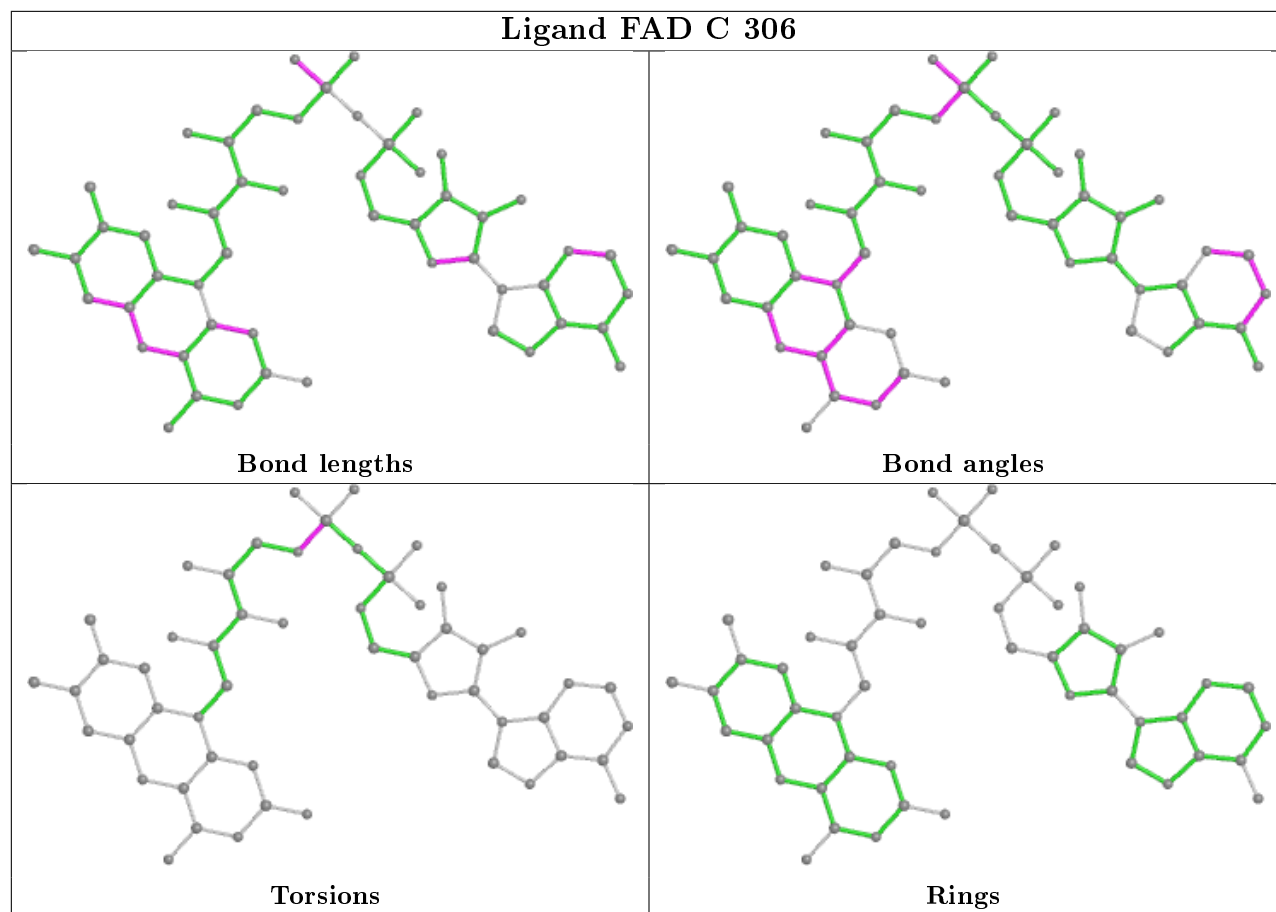
Mol	Chain	Res	Type	Atoms
6	B	311	BGC	O5-C5-C6-O6
6	B	311	BGC	C4-C5-C6-O6
3	C	306	FAD	C5'-O5'-P-O3P
3	A	306	FAD	C5'-O5'-P-O3P

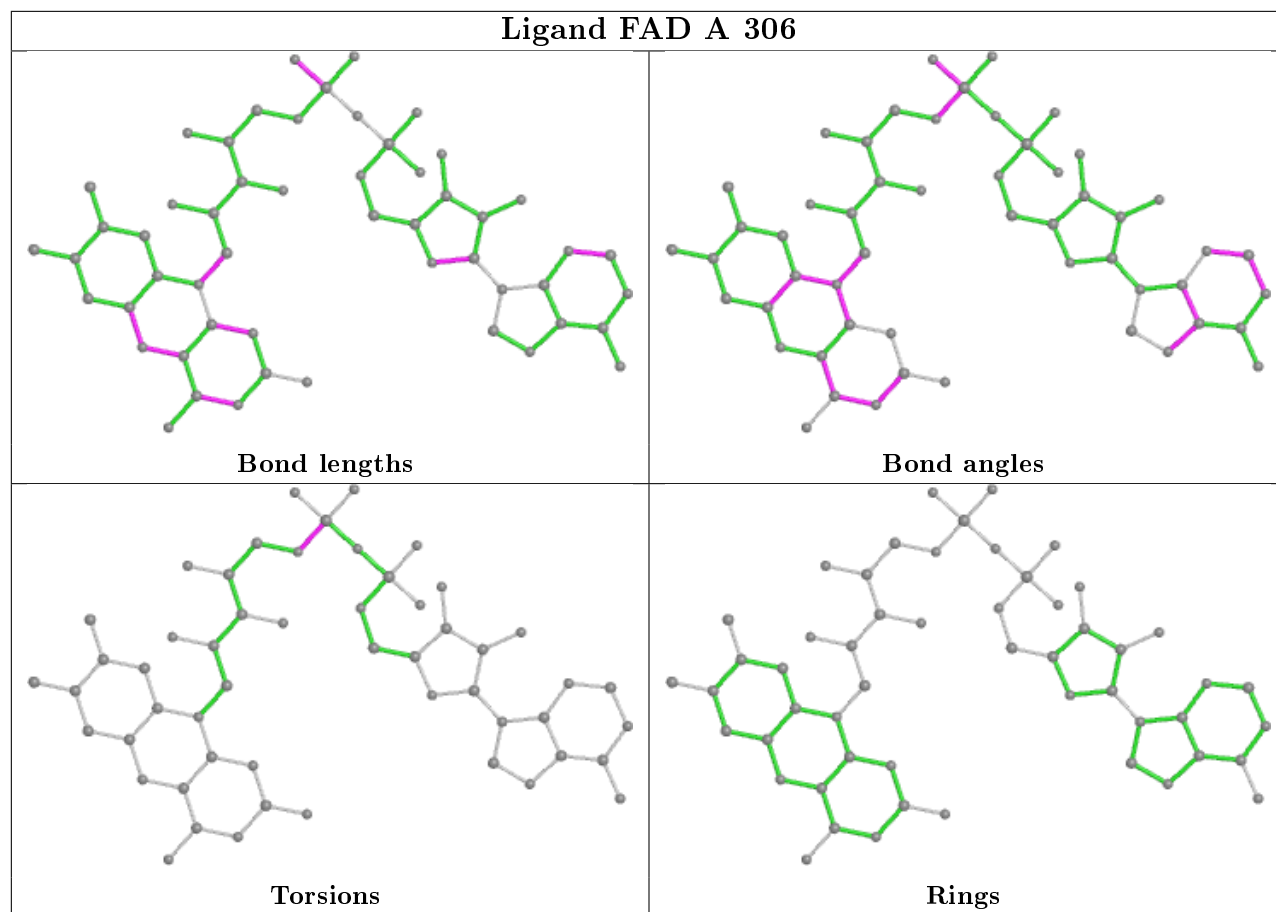
There are no ring outliers.

No monomer is involved in short contacts.

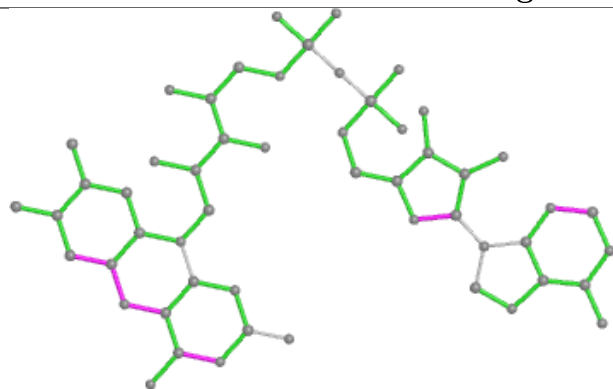
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



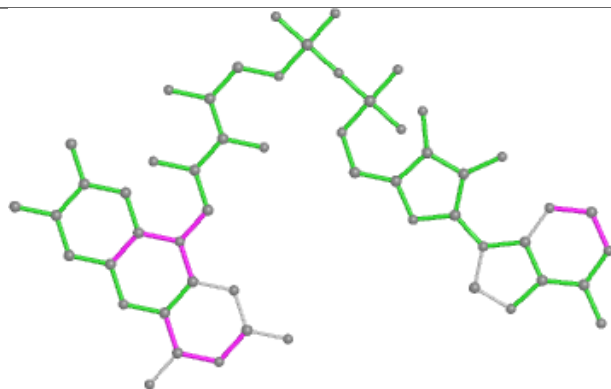




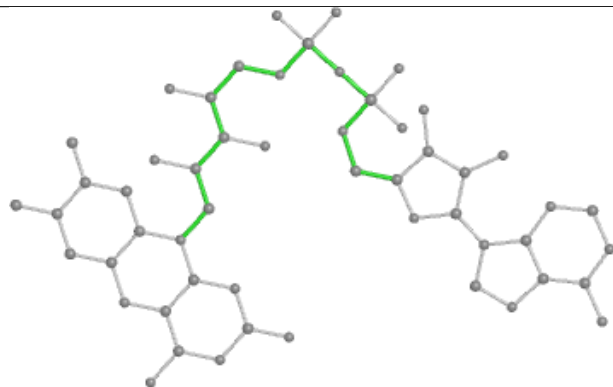
Ligand FAD F 306



Bond lengths



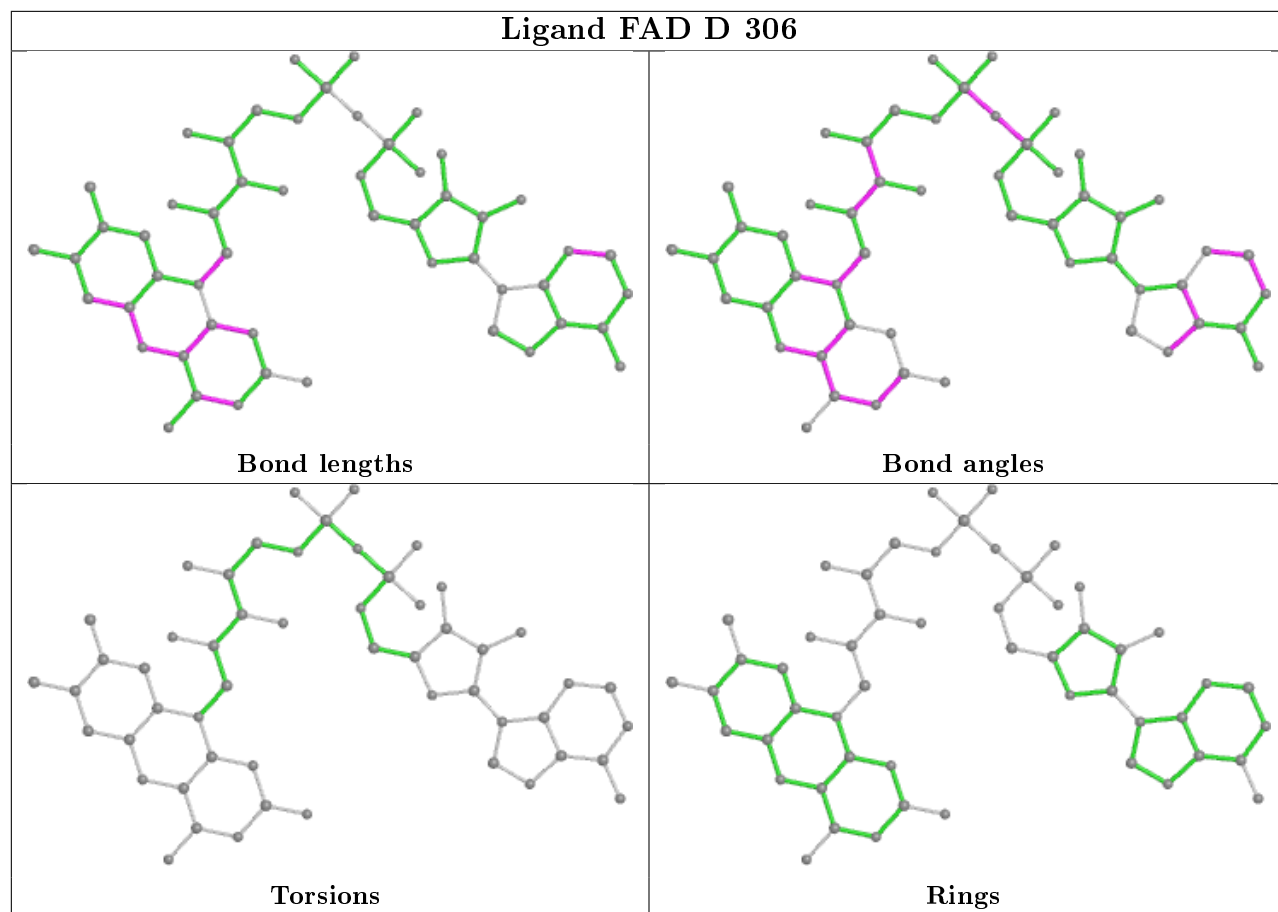
Bond angles

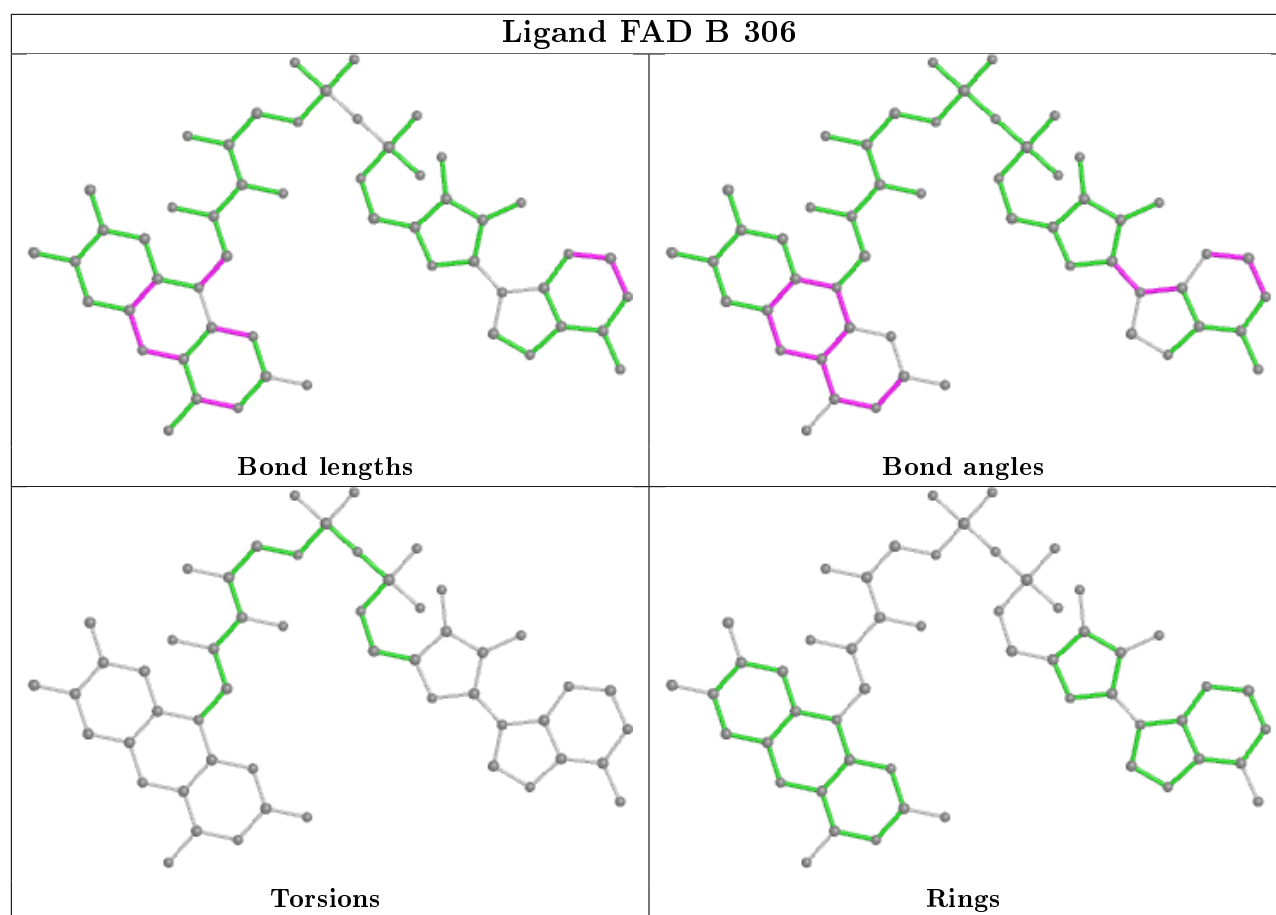


Torsions



Rings





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	299/308 (97%)	0.51	23 (7%) 13 14	7, 13, 28, 38	2 (0%)
1	B	305/308 (99%)	0.63	40 (13%) 3 3	9, 16, 31, 49	2 (0%)
1	C	292/308 (94%)	0.36	24 (8%) 11 13	9, 16, 28, 38	1 (0%)
1	D	301/308 (97%)	0.51	29 (9%) 8 10	8, 15, 29, 45	0
1	E	288/308 (93%)	0.75	42 (14%) 2 2	10, 19, 34, 42	3 (1%)
1	F	297/308 (96%)	0.33	21 (7%) 16 17	8, 14, 27, 48	1 (0%)
All	All	1782/1848 (96%)	0.51	179 (10%) 7 9	7, 15, 30, 49	9 (0%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	140	CYS	10.0
1	B	240	ASN	9.7
1	C	261	VAL	9.2
1	B	261	VAL	8.8
1	F	240	ASN	7.9
1	A	86	LEU	7.8
1	C	84	VAL	7.5
1	C	82	TYR	7.5
1	D	140	CYS	7.2
1	F	242	THR	7.1
1	A	88	GLN	7.0
1	D	240	ASN	6.9
1	D	261	VAL	6.9
1	E	261	VAL	6.7
1	B	242	THR	6.4
1	E	53	LEU	6.4
1	E	281[A]	HIS	6.2
1	B	239	LYS	6.0
1	F	86	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	F	241	SER	5.7
1	A	-3	GLY	5.6
1	E	84	VAL	5.4
1	B	260	GLU	5.4
1	D	239	LYS	5.3
1	A	89	SER	5.3
1	D	260	GLU	5.2
1	E	83	ILE	5.0
1	E	100	LEU	5.0
1	F	281	HIS	4.8
1	C	99	PRO	4.8
1	B	86	LEU	4.6
1	D	281	HIS	4.6
1	B	241	SER	4.5
1	E	98	PHE	4.5
1	F	238	ASP	4.5
1	E	82	TYR	4.4
1	A	240	ASN	4.4
1	F	239	LYS	4.4
1	A	242	THR	4.3
1	B	238	ASP	4.3
1	E	111	ASP	4.2
1	B	95	PHE	4.2
1	E	242	THR	4.1
1	C	81	TYR	4.1
1	E	170	PHE	4.0
1	D	241	SER	4.0
1	E	279	ASN	3.9
1	D	88	GLN	3.9
1	D	86	LEU	3.9
1	D	242	THR	3.8
1	C	304	LYS	3.8
1	D	53	LEU	3.8
1	A	70	LEU	3.8
1	A	87	SER	3.7
1	E	260	GLU	3.6
1	B	88	GLN	3.6
1	B	173	HIS	3.6
1	A	281[A]	HIS	3.5
1	B	266	PRO	3.5
1	A	265	GLU	3.5
1	C	53	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	242	THR	3.4
1	B	304	LYS	3.4
1	A	71	LEU	3.4
1	E	142	THR	3.4
1	E	274	LEU	3.3
1	C	83	ILE	3.3
1	A	99	PRO	3.2
1	B	84	VAL	3.2
1	D	85	LYS	3.2
1	E	81	TYR	3.2
1	C	239	LYS	3.2
1	E	79	TRP	3.2
1	F	304	LYS	3.1
1	D	238	ASP	3.1
1	B	302	LYS	3.1
1	F	-3	GLY	3.1
1	A	201	ILE	3.1
1	F	69	VAL	3.1
1	B	69	VAL	3.1
1	D	69	VAL	3.1
1	E	240	ASN	3.0
1	B	93	GLY	2.9
1	C	98	PHE	2.9
1	B	82	TYR	2.9
1	D	93	GLY	2.9
1	F	265	GLU	2.9
1	B	265	GLU	2.9
1	A	69	VAL	2.9
1	E	0	VAL	2.9
1	A	266	PRO	2.9
1	B	245	LYS	2.8
1	C	302	LYS	2.8
1	E	101	THR	2.8
1	B	70	LEU	2.8
1	C	260	GLU	2.8
1	E	110	HIS	2.8
1	A	161	VAL	2.8
1	F	243	PRO	2.8
1	B	91	PHE	2.8
1	B	85	LYS	2.8
1	E	278	GLU	2.8
1	D	91	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	87	SER	2.8
1	C	54	ASN	2.7
1	A	304	LYS	2.7
1	C	281	HIS	2.7
1	D	111	ASP	2.7
1	E	183	ASN	2.7
1	B	161	VAL	2.7
1	B	71	LEU	2.7
1	F	70	LEU	2.7
1	B	97	ARG	2.7
1	D	97	ARG	2.7
1	E	137	ARG	2.7
1	E	99	PRO	2.7
1	D	265	GLU	2.6
1	E	239	LYS	2.6
1	A	238[A]	ASP	2.6
1	E	139	LYS	2.6
1	C	240	ASN	2.6
1	E	54	ASN	2.6
1	B	152	GLN	2.6
1	B	0	VAL	2.6
1	E	282[A]	GLU	2.5
1	E	152	GLN	2.5
1	E	2	ARG	2.5
1	D	84	VAL	2.5
1	F	0	VAL	2.5
1	C	170	PHE	2.5
1	D	243	PRO	2.5
1	B	25	ASP	2.5
1	B	170	PHE	2.5
1	D	170	PHE	2.5
1	D	266	PRO	2.4
1	B	281	HIS	2.4
1	D	95	PHE	2.4
1	A	75	LEU	2.3
1	E	151	LEU	2.3
1	C	161	VAL	2.3
1	F	162	ILE	2.3
1	E	103[A]	LEU	2.3
1	B	263	LYS	2.3
1	B	226[A]	VAL	2.3
1	C	263	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	161	VAL	2.2
1	B	81	TYR	2.2
1	A	85	LYS	2.2
1	B	193	LEU	2.2
1	E	149	THR	2.2
1	D	96	HIS	2.2
1	E	145	GLU	2.1
1	B	201	ILE	2.1
1	E	259	ASN	2.1
1	B	23	GLU	2.1
1	C	243	PRO	2.1
1	A	73	LEU	2.1
1	A	205	LEU	2.1
1	C	257	LYS	2.1
1	F	294	LYS	2.1
1	B	243	PRO	2.1
1	C	241	SER	2.1
1	B	21	ALA	2.1
1	A	204	PHE	2.1
1	E	226[A]	VAL	2.1
1	F	266	PRO	2.1
1	D	267	ILE	2.1
1	B	96	HIS	2.0
1	E	138	ASP	2.0
1	E	238	ASP	2.0
1	E	154	PHE	2.0
1	C	70	LEU	2.0
1	D	70	LEU	2.0
1	D	71	LEU	2.0
1	F	71	LEU	2.0
1	C	266	PRO	2.0
1	F	260	GLU	2.0
1	E	144	ALA	2.0
1	D	152	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

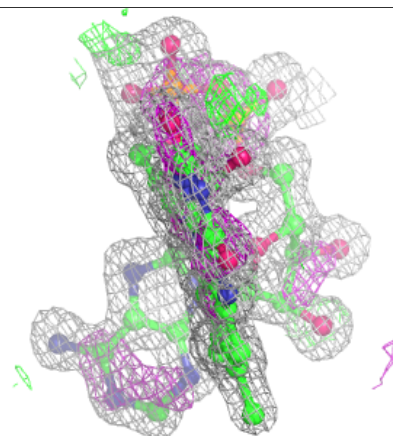
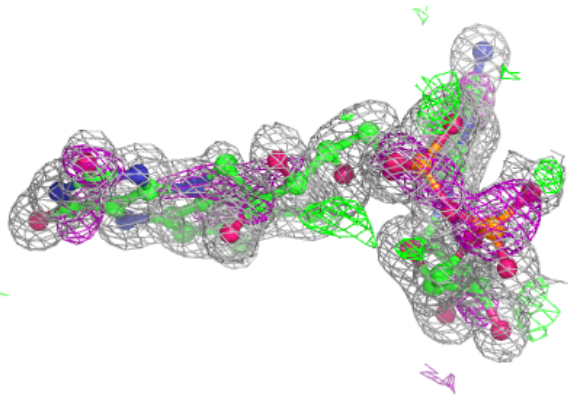
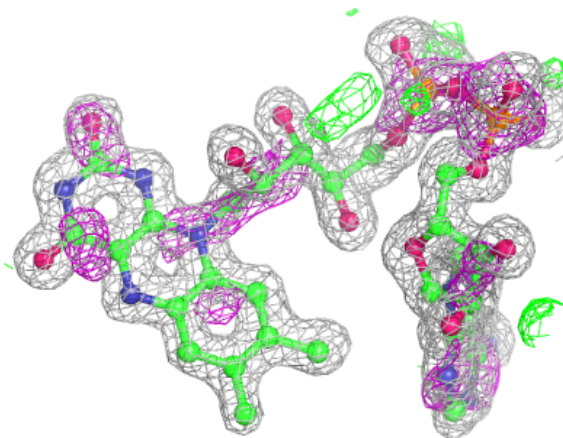
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	BGC	B	311	12/12	0.74	0.18	25,30,32,33	12
4	MG	F	309	1/1	0.82	0.11	23,23,23,23	1
5	SO4	F	311	5/5	0.86	0.18	21,23,24,25	5
4	MG	A	309	1/1	0.88	0.19	20,20,20,20	1
3	FAD	E	306	53/53	0.92	0.16	15,20,25,29	0
4	MG	F	310	1/1	0.92	0.10	15,15,15,15	1
3	FAD	C	306	53/53	0.94	0.10	12,15,20,22	0
5	SO4	B	310	5/5	0.95	0.09	27,27,28,29	5
5	SO4	D	308	5/5	0.95	0.09	25,26,26,26	5
4	MG	A	308	1/1	0.95	0.12	14,14,14,14	1
4	MG	B	309	1/1	0.95	0.38	17,17,17,17	1
3	FAD	B	306	53/53	0.95	0.10	11,17,22,23	0
3	FAD	D	306	53/53	0.96	0.07	9,14,20,24	0
3	FAD	A	306	53/53	0.96	0.08	9,13,17,22	0
4	MG	F	308	1/1	0.97	0.12	15,15,15,15	1
4	MG	B	308	1/1	0.97	0.09	20,20,20,20	1
5	SO4	D	309	5/5	0.97	0.06	28,28,29,29	5
3	FAD	F	306	53/53	0.97	0.07	9,13,17,23	0
2	POP	B	305	9/9	0.99	0.07	9,10,12,13	0
2	POP	C	305	9/9	0.99	0.06	9,10,11,11	0
2	POP	E	305	9/9	0.99	0.05	12,12,13,14	0
2	POP	A	305	9/9	1.00	0.10	8,8,9,10	0
2	POP	F	305	9/9	1.00	0.07	8,8,10,11	0
4	MG	D	307	1/1	1.00	0.06	8,8,8,8	0
4	MG	B	307	1/1	1.00	0.09	9,9,9,9	0
4	MG	F	307	1/1	1.00	0.09	7,7,7,7	0
4	MG	C	307	1/1	1.00	0.04	9,9,9,9	0
4	MG	E	307	1/1	1.00	0.04	11,11,11,11	0
4	MG	A	307	1/1	1.00	0.09	7,7,7,7	0
2	POP	D	305	9/9	1.00	0.08	8,9,9,10	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.

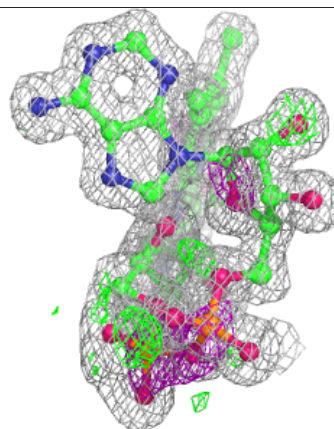
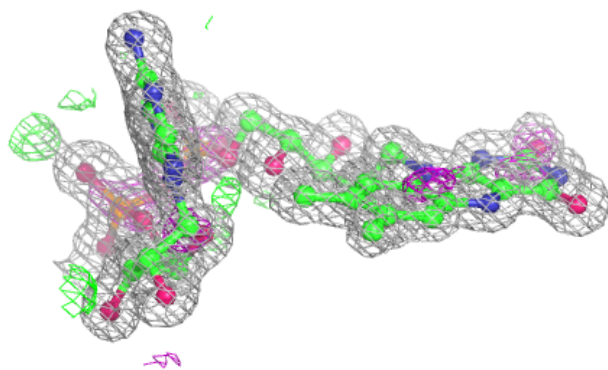
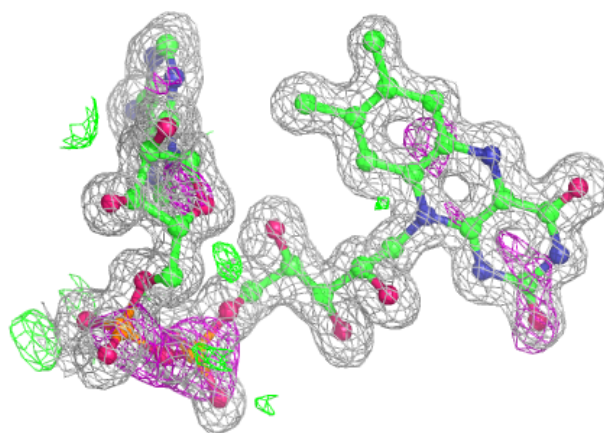
Electron density around FAD E 306:

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



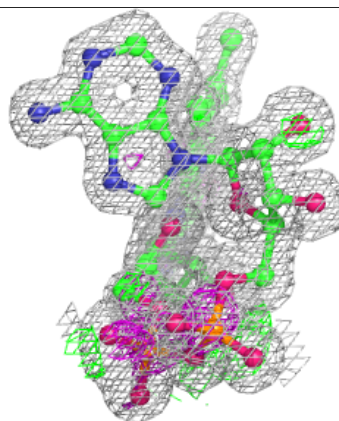
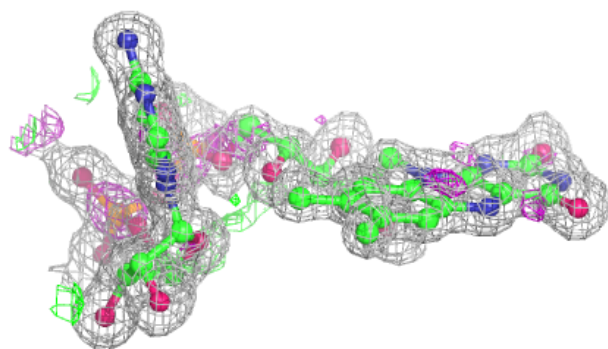
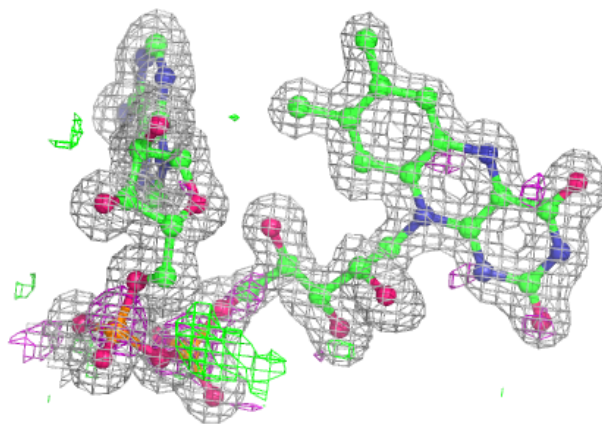
Electron density around FAD C 306:

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



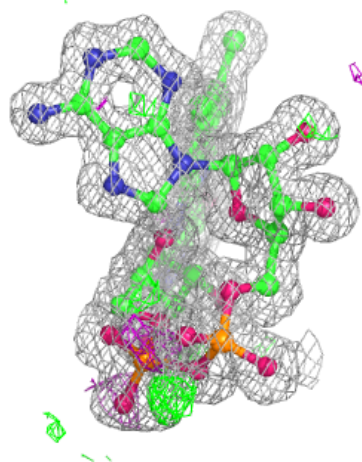
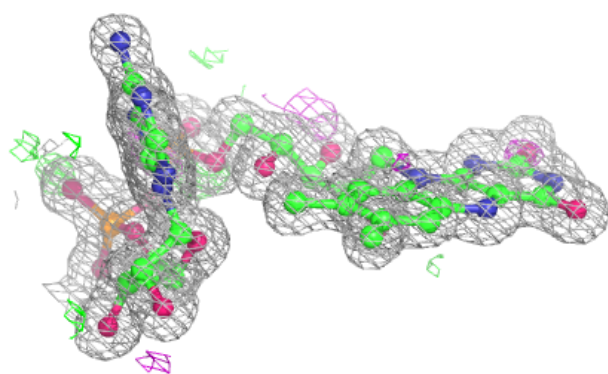
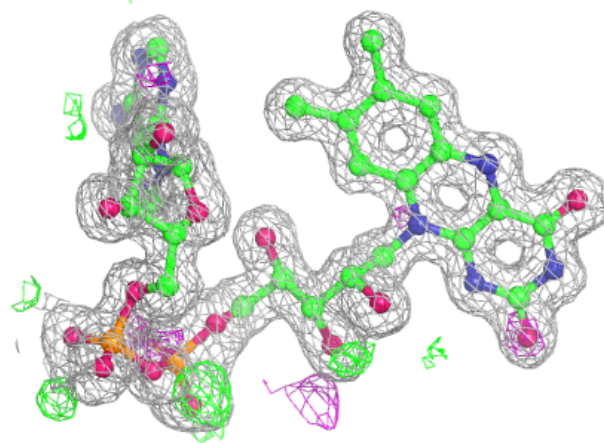
Electron density around FAD B 306:

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



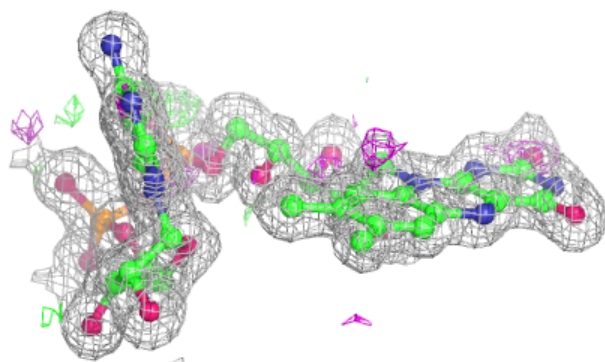
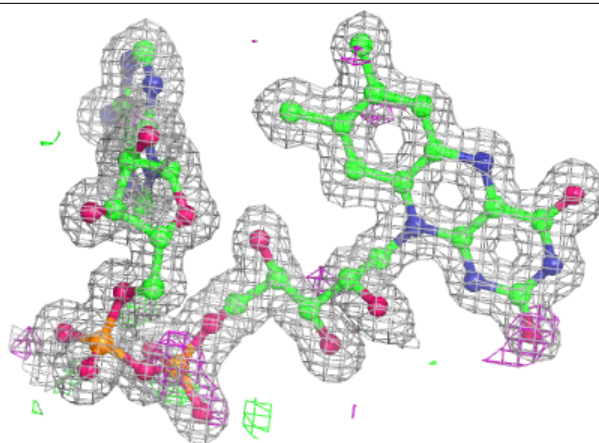
Electron density around FAD D 306:

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



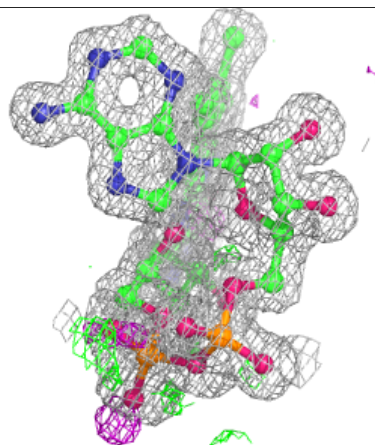
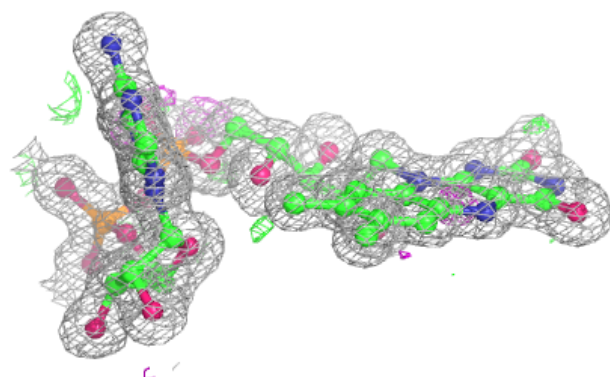
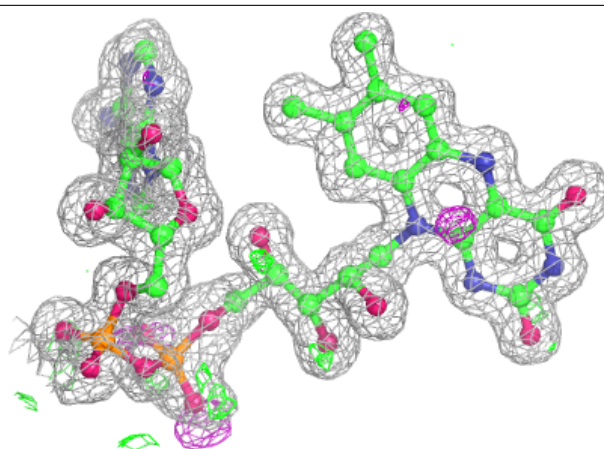
Electron density around FAD A 306:

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



Electron density around FAD F 306:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.