wwPDB X-ray Structure Validation Summary Report (i)

Jul 6, 2023 – 06:01 pm BST

PDB ID	:	8AQ8
Title	:	FAD-dependent monooxygenase from Stenotrophomonas maltophilia
Authors	:	Maly, M.; Kolenko, P.; Duskova, J.; Skalova, T.; Dohnalek, J.
Deposited on	:	2022-08-11
Resolution	:	1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

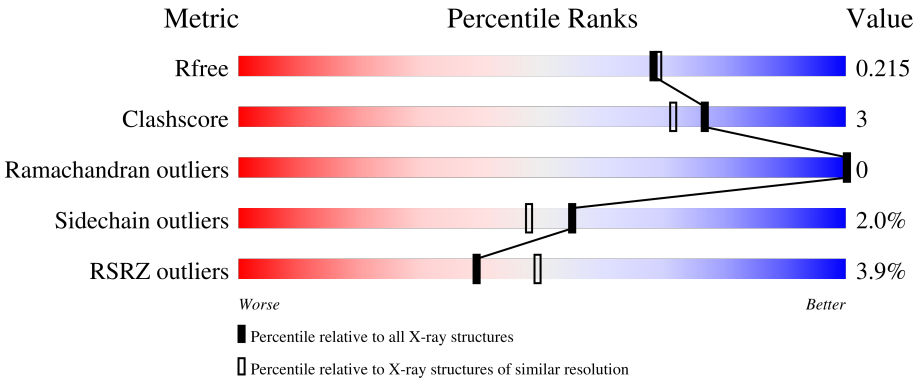
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	AAA	366	4% 86% 7% • 6%
1	BBB	366	4% 89% 5% 6%
1	CCC	366	4% 86% 7% 7%
1	DDD	366	2% 85% 7% • 7%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11859 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.

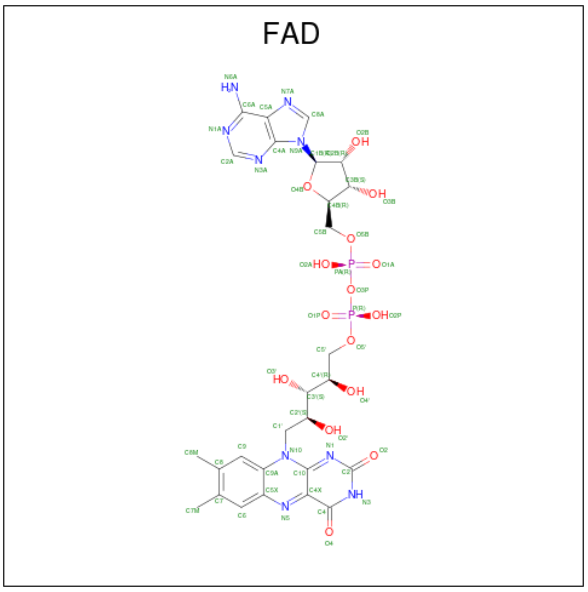
- Molecule 1 is a protein called Monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	344	Total	C	N	O	S	0	6	0
			2635	1650	483	487	15			
1	BBB	343	Total	C	N	O	S	0	4	0
			2609	1636	478	480	15			
1	CCC	342	Total	C	N	O	S	0	5	0
			2613	1638	480	481	14			
1	DDD	339	Total	C	N	O	S	0	5	0
			2596	1628	479	475	14			

There are 16 discrepancies between the modelled and reference sequences:

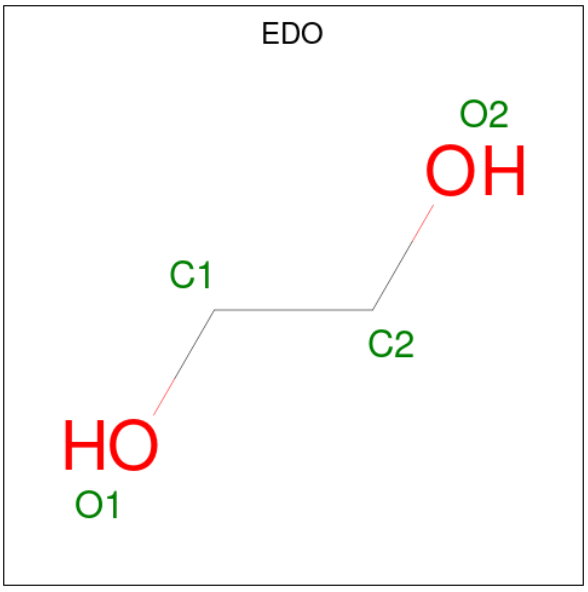
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	GLY	-	expression tag	UNP A0A2Y9UCL1
AAA	0	HIS	-	expression tag	UNP A0A2Y9UCL1
AAA	154	ILE	MET	variant	UNP A0A2Y9UCL1
AAA	283	THR	ALA	variant	UNP A0A2Y9UCL1
BBB	-1	GLY	-	expression tag	UNP A0A2Y9UCL1
BBB	0	HIS	-	expression tag	UNP A0A2Y9UCL1
BBB	154	ILE	MET	variant	UNP A0A2Y9UCL1
BBB	283	THR	ALA	variant	UNP A0A2Y9UCL1
CCC	-1	GLY	-	expression tag	UNP A0A2Y9UCL1
CCC	0	HIS	-	expression tag	UNP A0A2Y9UCL1
CCC	154	ILE	MET	variant	UNP A0A2Y9UCL1
CCC	283	THR	ALA	variant	UNP A0A2Y9UCL1
DDD	-1	GLY	-	expression tag	UNP A0A2Y9UCL1
DDD	0	HIS	-	expression tag	UNP A0A2Y9UCL1
DDD	154	ILE	MET	variant	UNP A0A2Y9UCL1
DDD	283	THR	ALA	variant	UNP A0A2Y9UCL1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



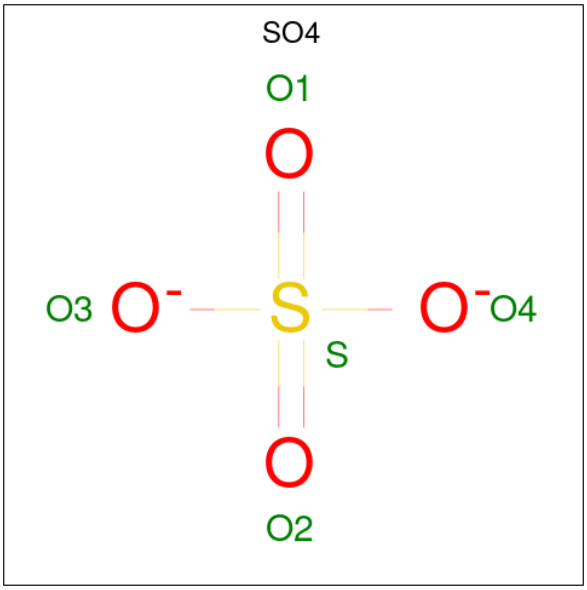
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	BBB	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	CCC	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	DDD	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



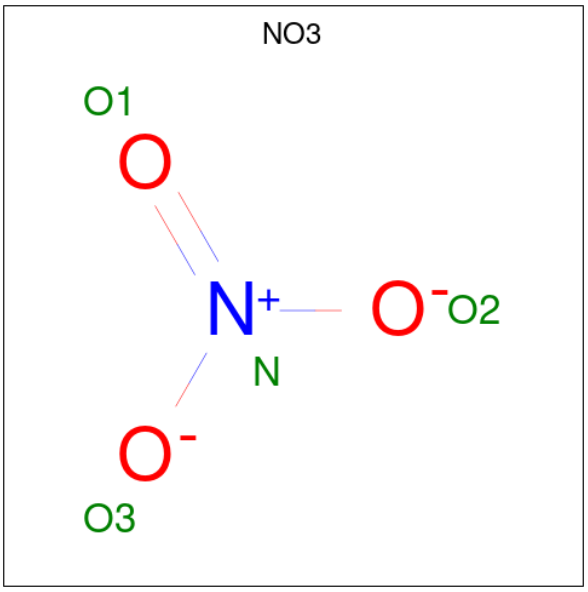
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	DDD	1	Total C O 4 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



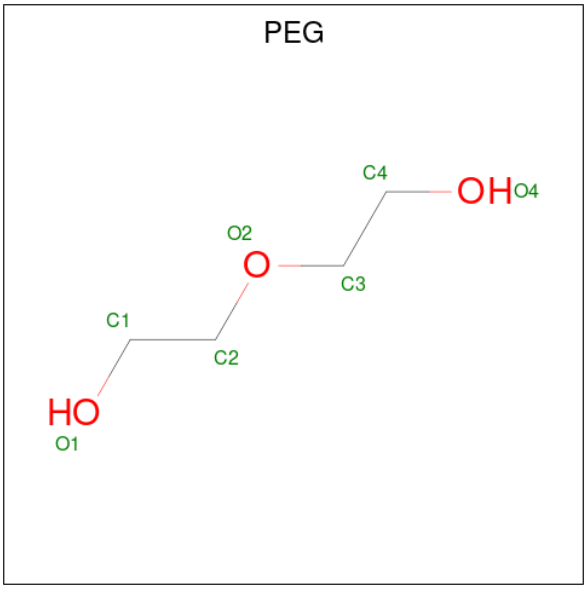
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total O S 5 4 1	0	0
4	AAA	1	Total O S 5 4 1	0	0

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total N O 4 1 3	0	0
5	BBB	1	Total N O 4 1 3	0	0
5	CCC	1	Total N O 4 1 3	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	DDD	1	Total C O 7 4 3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total Cl 1 1	0	0
7	BBB	1	Total Cl 1 1	0	0
7	CCC	1	Total Cl 1 1	0	0
7	DDD	1	Total Cl 1 1	0	0

- Molecule 8 is water.

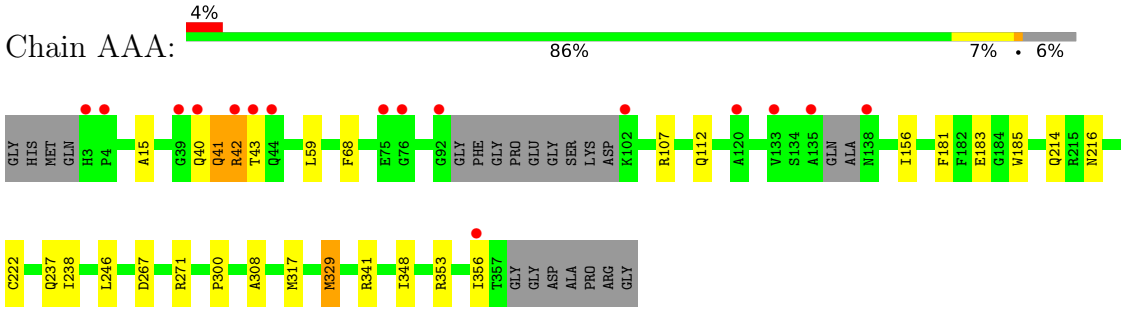
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	287	Total O 292 292	0	6
8	BBB	266	Total O 268 268	0	2
8	CCC	296	Total O 302 302	0	6
8	DDD	262	Total O 268 268	0	6

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.

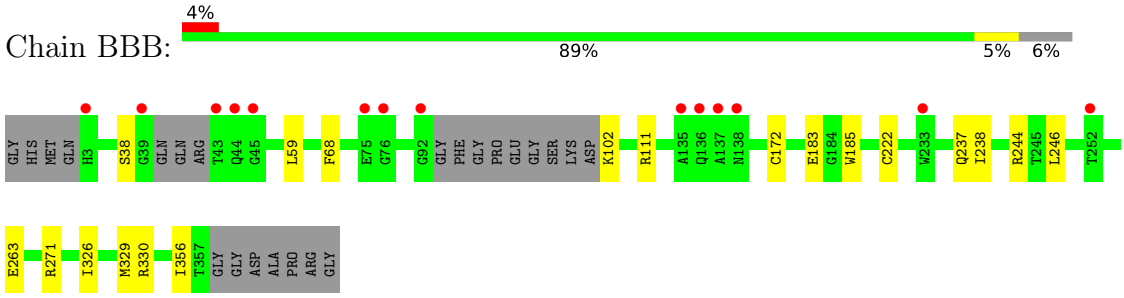
• Molecule 1: Monooxygenase

Chain AAA:



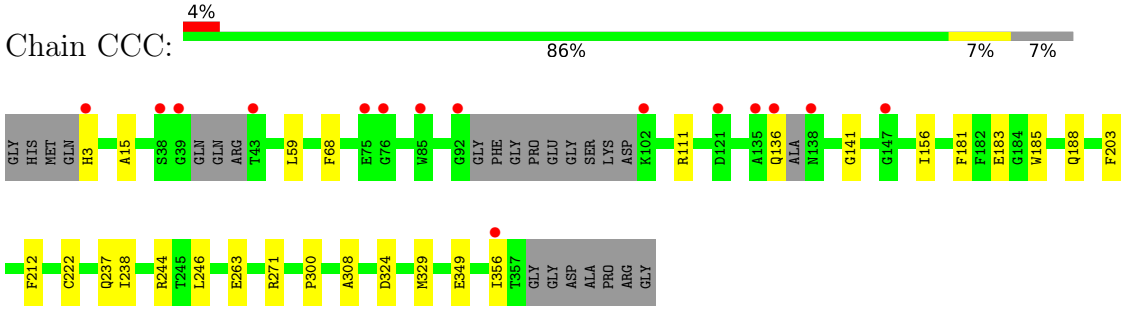
• Molecule 1: Monooxygenase

Chain BBB:



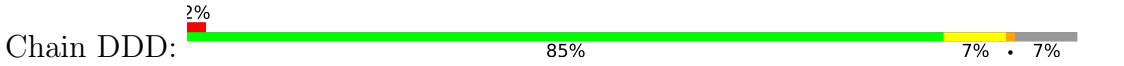
• Molecule 1: Monooxygenase

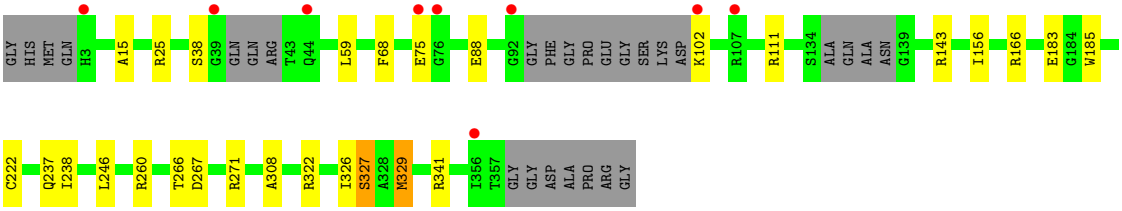
Chain CCC:



• Molecule 1: Monooxygenase

Chain DDD:




GLY HIS MET GLN H3 A15 R25 S38 G39 GLN GLN ARG T43 Q44 L59 F68 E75 G76 E88 G92 GLY PHE GLY PRO GLU GLY SER LYS ASP K102 R107 R111 S134 ALA GLN ALA ASN G139 R143 I156 R166 E183 G184 W185
C222 Q237 I238 L246 R260 T266 D267 R271 A308 R322 I326 S327 A328 M329 R341 I356 T357 GLY GLY ASP ALA PRO ARG GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.93Å 160.53Å 95.56Å 90.00° 95.91° 90.00°	Depositor
Resolution (Å)	48.26 – 1.95 48.21 – 1.95	Depositor EDS
% Data completeness (in resolution range)	85.3 (48.26-1.95) 85.3 (48.21-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.200 , 0.241 0.208 , 0.215	Depositor DCC
R_{free} test set	4917 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11859	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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 49.87 % 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 7.0162e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FAD, CL, PEG, NO3, EDO, SO4

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	AAA	0.70	0/2703	0.85	0/3669
1	BBB	0.70	0/2674	0.84	0/3631
1	CCC	0.71	0/2680	0.84	0/3637
1	DDD	0.69	0/2660	0.84	1/3610 (0.0%)
All	All	0.70	0/10717	0.84	1/14547 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DDD	166	ARG	NE-CZ-NH2	-5.32	117.64	120.30

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	AAA	2635	0	2597	22	0
1	BBB	2609	0	2575	8	0
1	CCC	2613	0	2579	17	0
1	DDD	2596	0	2567	17	0
2	AAA	53	0	31	1	0
2	BBB	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	53	0	31	1	0
2	DDD	53	0	31	0	0
3	AAA	8	0	12	0	0
3	BBB	4	0	6	0	0
3	CCC	8	0	12	0	0
3	DDD	4	0	6	0	0
4	AAA	10	0	0	0	0
5	AAA	4	0	0	0	0
5	BBB	4	0	0	0	0
5	CCC	4	0	0	0	0
6	AAA	7	0	10	1	0
6	DDD	7	0	10	0	0
7	AAA	1	0	0	1	0
7	BBB	1	0	0	0	0
7	CCC	1	0	0	1	0
7	DDD	1	0	0	0	0
8	AAA	292	0	0	8	0
8	BBB	268	0	0	1	0
8	CCC	302	0	0	4	0
8	DDD	268	0	0	5	0
All	All	11859	0	10498	64	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.

The worst 5 of 64 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:CCC:188:GLN:HB2	8:CCC:698:HOH:O	1.83	0.77
1:DDD:237:GLN:HB3	1:DDD:246:LEU:HD13	1.64	0.76
1:BBB:237:GLN:HB3	1:BBB:246:LEU:HD13	1.67	0.75
1:AAA:237:GLN:HB3	1:AAA:246:LEU:HD13	1.72	0.71
1:CCC:237:GLN:HB3	1:CCC:246:LEU:HD13	1.72	0.71

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	AAA	344/366 (94%)	333 (97%)	11 (3%)	0	100	100
1	BBB	341/366 (93%)	331 (97%)	10 (3%)	0	100	100
1	CCC	339/366 (93%)	331 (98%)	8 (2%)	0	100	100
1	DDD	336/366 (92%)	328 (98%)	8 (2%)	0	100	100
All	All	1360/1464 (93%)	1323 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	AAA	266/273 (97%)	262 (98%)	4 (2%)	65	60
1	BBB	262/273 (96%)	255 (97%)	7 (3%)	44	34
1	CCC	263/273 (96%)	261 (99%)	2 (1%)	81	80
1	DDD	261/273 (96%)	253 (97%)	8 (3%)	40	28
All	All	1052/1092 (96%)	1031 (98%)	21 (2%)	55	48

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	102	LYS
1	DDD	267	ASP
1	DDD	329	MET

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Mol	Chain	Res	Type
1	DDD	326	ILE
1	DDD	266	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
2	FAD	AAA	401	-	53,58,58	0.70	0	68,89,89	0.77	0
3	EDO	AAA	402	-	3,3,3	0.24	0	2,2,2	0.20	0
5	NO3	AAA	406	-	1,3,3	0.11	0	0,3,3	-	-
4	SO4	AAA	404	-	4,4,4	0.31	0	6,6,6	0.06	0
6	PEG	DDD	403	-	6,6,6	0.31	0	5,5,5	0.19	0
2	FAD	DDD	401	-	53,58,58	0.83	2 (3%)	68,89,89	0.82	1 (1%)
3	EDO	AAA	405	-	3,3,3	0.11	0	2,2,2	0.08	0
3	EDO	CCC	402	-	3,3,3	0.20	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	DDD	402	-	3,3,3	0.09	0	2,2,2	0.33	0
2	FAD	BBB	401	-	53,58,58	0.71	1 (1%)	68,89,89	0.82	1 (1%)
4	SO4	AAA	403	-	4,4,4	0.37	0	6,6,6	0.41	0
5	NO3	BBB	403	-	1,3,3	0.29	0	0,3,3	-	-
5	NO3	CCC	403	-	1,3,3	0.19	0	0,3,3	-	-
3	EDO	CCC	404	-	3,3,3	0.37	0	2,2,2	0.03	0
6	PEG	AAA	407	-	6,6,6	0.56	0	5,5,5	0.35	0
2	FAD	CCC	401	-	53,58,58	0.77	0	68,89,89	0.83	2 (2%)
3	EDO	BBB	402	-	3,3,3	0.47	0	2,2,2	0.46	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	FAD	AAA	401	-	-	2/30/50/50	0/6/6/6
3	EDO	AAA	402	-	-	0/1/1/1	-
6	PEG	DDD	403	-	-	1/4/4/4	-
2	FAD	DDD	401	-	-	1/30/50/50	0/6/6/6
3	EDO	AAA	405	-	-	1/1/1/1	-
3	EDO	CCC	402	-	-	0/1/1/1	-
3	EDO	DDD	402	-	-	0/1/1/1	-
2	FAD	BBB	401	-	-	4/30/50/50	0/6/6/6
6	PEG	AAA	407	-	-	0/4/4/4	-
3	EDO	CCC	404	-	-	0/1/1/1	-
2	FAD	CCC	401	-	-	1/30/50/50	0/6/6/6
3	EDO	BBB	402	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	401	FAD	C1'-C2'	-2.20	1.49	1.52
2	DDD	401	FAD	C2-N1	-2.10	1.31	1.36
2	BBB	401	FAD	C8A-N7A	-2.03	1.31	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	401	FAD	C5A-C6A-N6A	2.54	124.21	120.35
2	CCC	401	FAD	C4-N3-C2	-2.08	121.80	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	401	FAD	C4-N3-C2	-2.05	121.85	125.64
2	CCC	401	FAD	O2P-P-O1P	2.03	122.28	112.24

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	401	FAD	PA-O3P-P-O5'
6	DDD	403	PEG	C1-C2-O2-C3
3	AAA	405	EDO	O1-C1-C2-O2
2	BBB	401	FAD	O2'-C2'-C3'-O3'
2	BBB	401	FAD	O2'-C2'-C3'-C4'

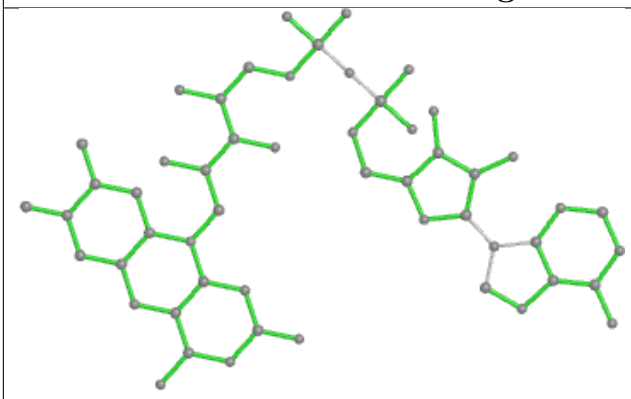
There are no ring outliers.

3 monomers are involved in 3 short contacts:

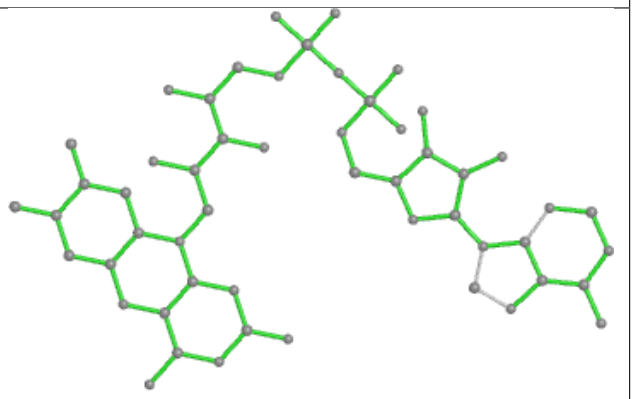
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	401	FAD	1	0
6	AAA	407	PEG	1	0
2	CCC	401	FAD	1	0

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 then 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.

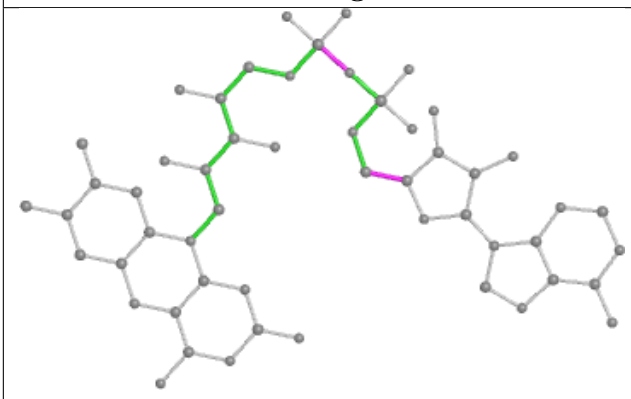
Ligand FAD AAA 401



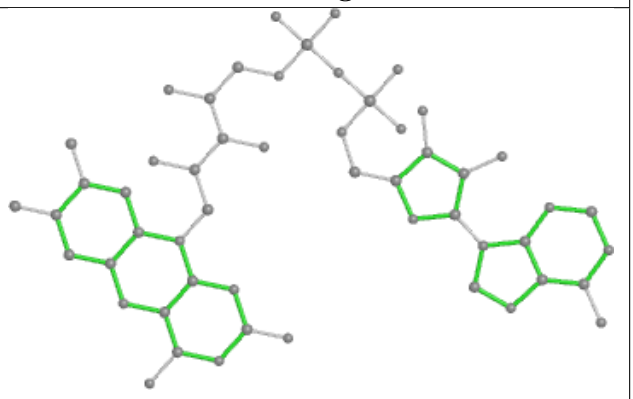
Bond lengths



Bond angles

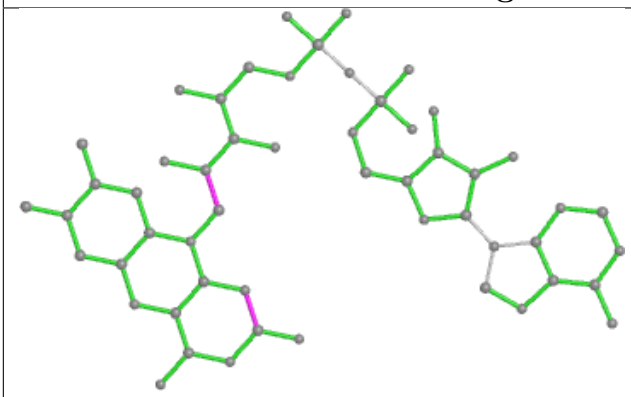


Torsions

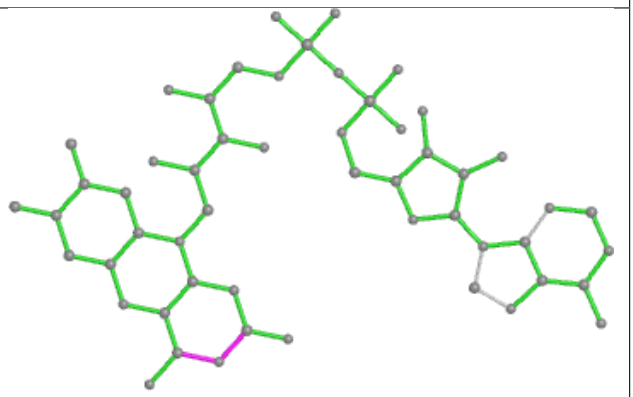


Rings

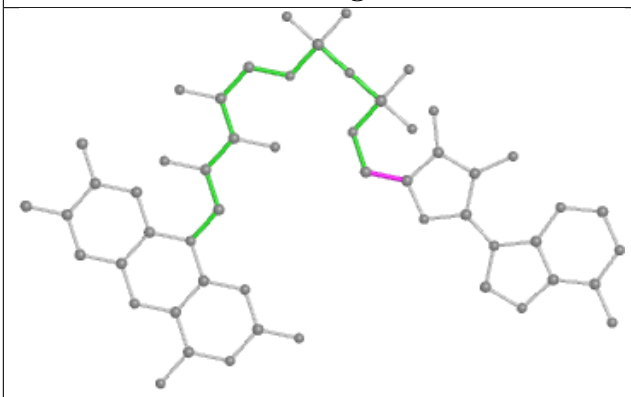
Ligand FAD DDD 401



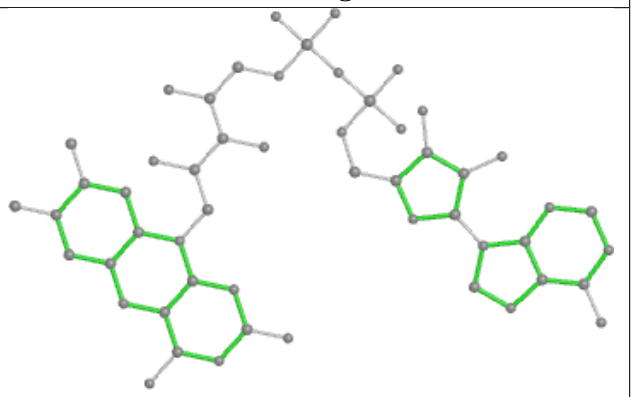
Bond lengths



Bond angles

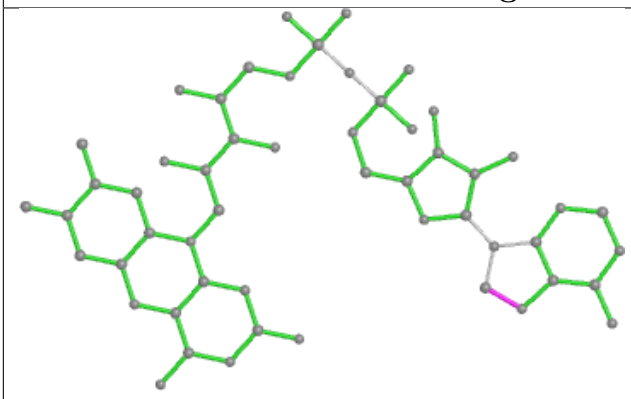


Torsions

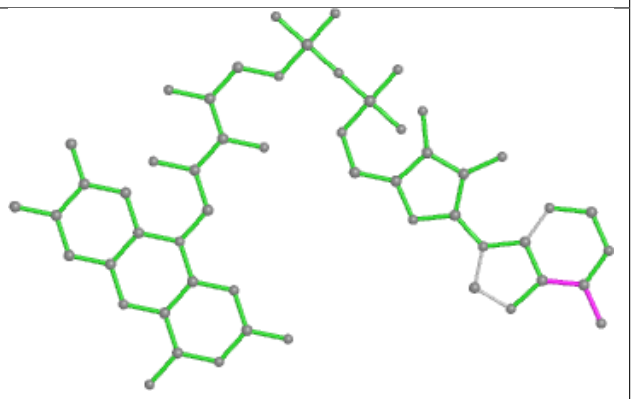


Rings

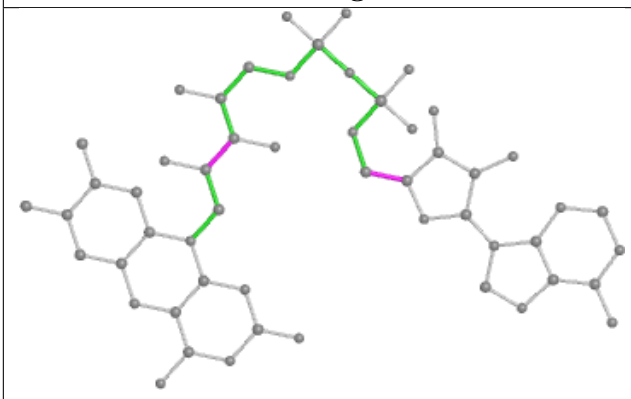
Ligand FAD BBB 401



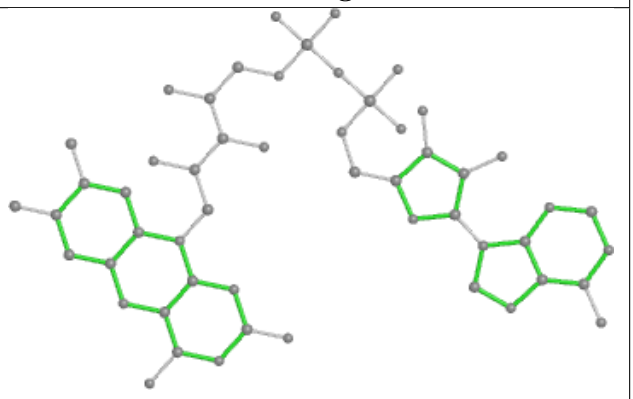
Bond lengths



Bond angles

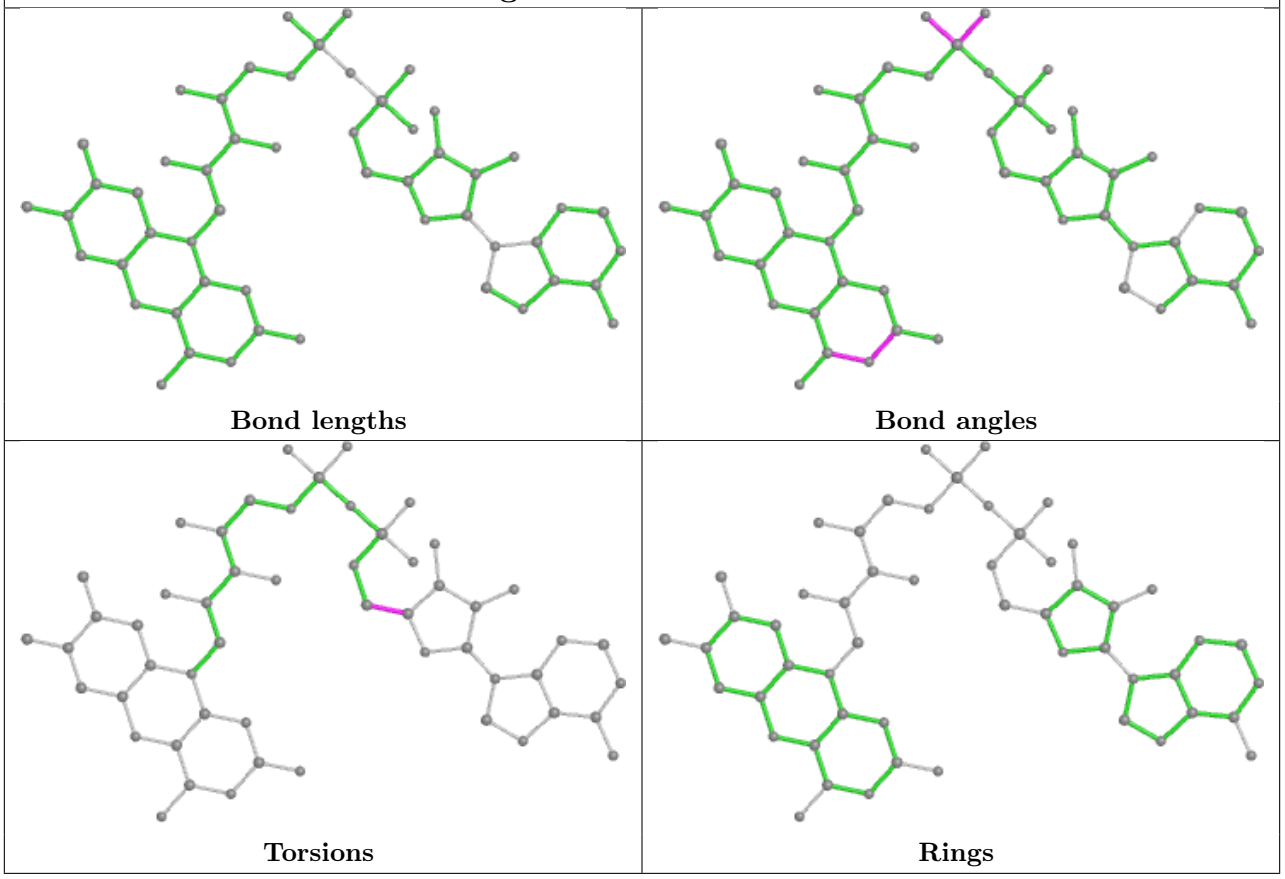


Torsions



Rings

Ligand FAD CCC 401



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, 95^{th} 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	AAA	344/366 (93%)	0.12	16 (4%)	31	41	14, 25, 61, 101	1 (0%)
1	BBB	343/366 (93%)	0.06	14 (4%)	37	46	13, 27, 58, 104	1 (0%)
1	CCC	342/366 (93%)	0.18	15 (4%)	34	44	15, 27, 61, 99	2 (0%)
1	DDD	339/366 (92%)	-0.00	9 (2%)	54	63	15, 27, 53, 82	1 (0%)
All	All	1368/1464 (93%)	0.09	54 (3%)	39	49	13, 26, 59, 104	5 (0%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	135	ALA	8.2
1	BBB	137	ALA	7.9
1	CCC	76	GLY	7.5
1	AAA	40	GLN	6.2
1	CCC	135	ALA	5.8

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

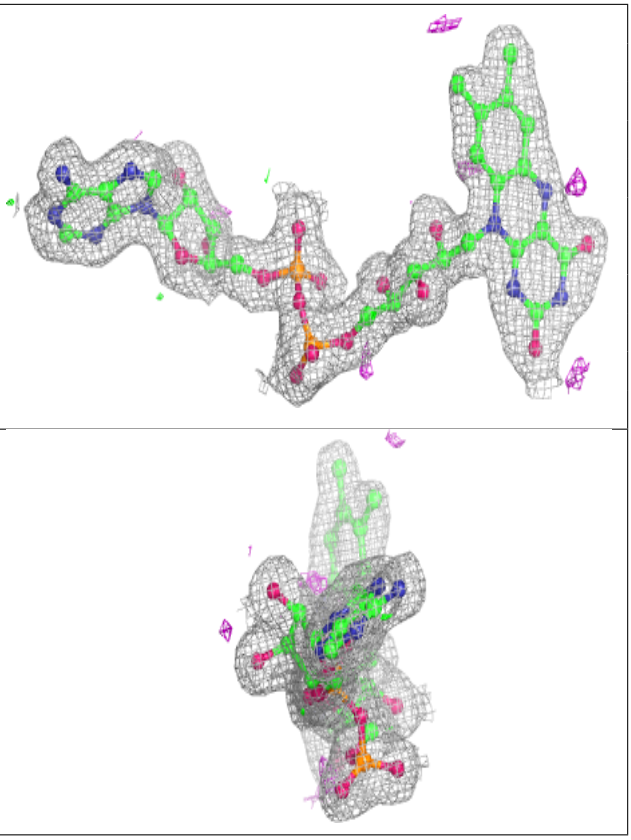
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	PEG	AAA	407	7/7	0.75	0.23	34,40,47,47	0
6	PEG	DDD	403	7/7	0.84	0.18	33,35,39,42	0
3	EDO	AAA	405	4/4	0.93	0.12	36,36,36,42	0
5	NO3	BBB	403	4/4	0.95	0.10	44,47,47,53	0
3	EDO	CCC	404	4/4	0.96	0.12	36,37,41,43	0
5	NO3	CCC	403	4/4	0.96	0.08	42,45,45,46	0
4	SO4	AAA	404	5/5	0.96	0.15	51,65,69,72	0
5	NO3	AAA	406	4/4	0.96	0.15	36,47,49,59	0
3	EDO	DDD	402	4/4	0.97	0.07	24,27,27,28	0
4	SO4	AAA	403	5/5	0.97	0.12	33,37,43,46	0
3	EDO	BBB	402	4/4	0.97	0.11	24,24,27,28	0
2	FAD	AAA	401	53/53	0.97	0.10	13,16,25,34	0
3	EDO	CCC	402	4/4	0.98	0.09	18,20,21,21	0
2	FAD	DDD	401	53/53	0.98	0.08	14,18,23,27	0
3	EDO	AAA	402	4/4	0.98	0.08	18,19,19,20	0
2	FAD	BBB	401	53/53	0.98	0.09	13,17,24,27	0
2	FAD	CCC	401	53/53	0.98	0.09	14,20,24,29	0
7	CL	AAA	408	1/1	0.99	0.09	22,22,22,22	0
7	CL	BBB	404	1/1	1.00	0.08	21,21,21,21	0
7	CL	CCC	405	1/1	1.00	0.09	21,21,21,21	0
7	CL	DDD	404	1/1	1.00	0.06	21,21,21,21	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.

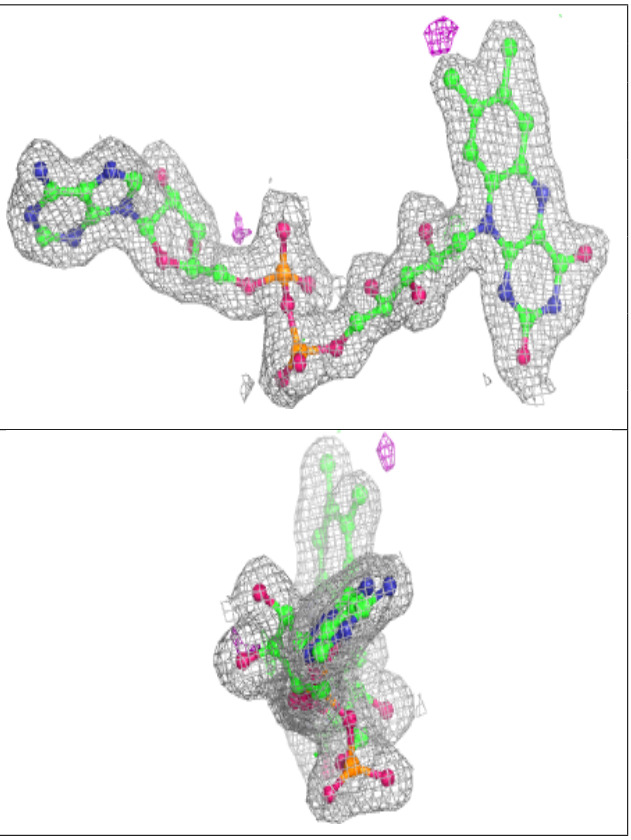
Electron density around FAD AAA 401:

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



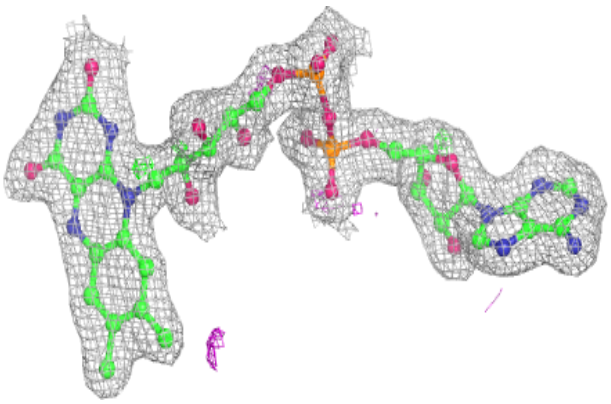
Electron density around FAD DDD 401:

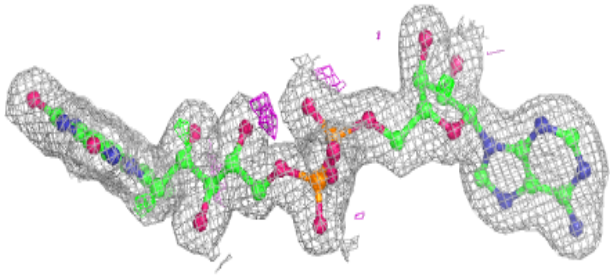
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

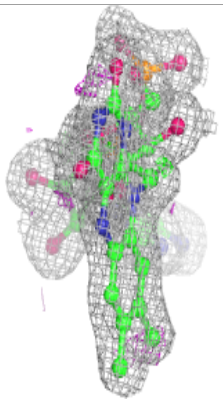


Electron density around FAD BBB 401:

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

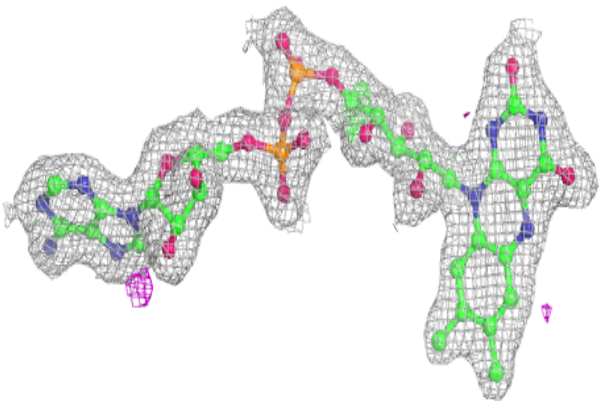


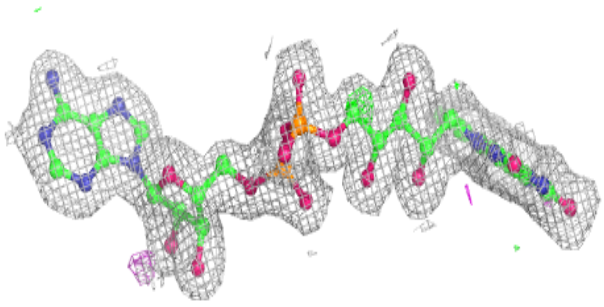


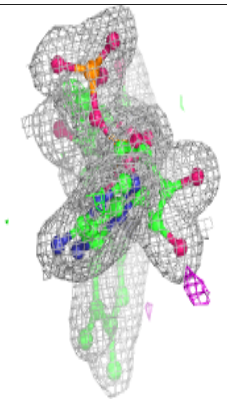


Electron density around FAD CCC 401:

$2mF_o$-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.