



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:41 PM UTC

PDB ID : 8AQ8 / pdb_00008aq8
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 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

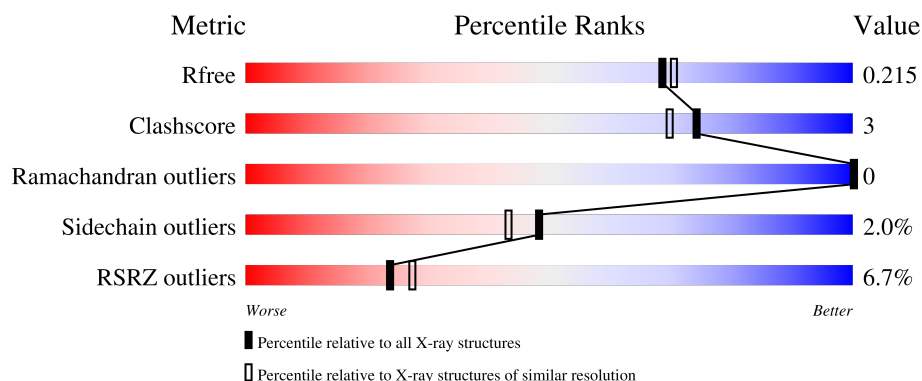
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 $\leq 5\%$. 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	AAA	366	6% 86% 7% 6%
1	BBB	366	6% 88% 6% 6%
1	CCC	366	7% 86% 8% 7%
1	DDD	366	6% 84% 8% 7%

2 Entry composition

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.

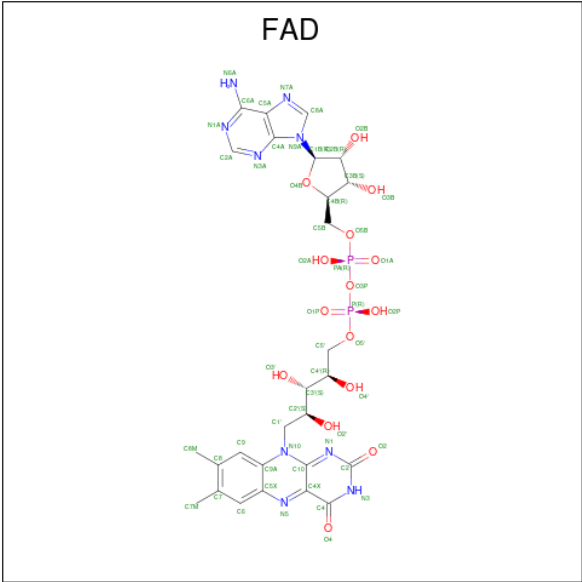
- Molecule 1 is a protein called Monooxygenase.

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:

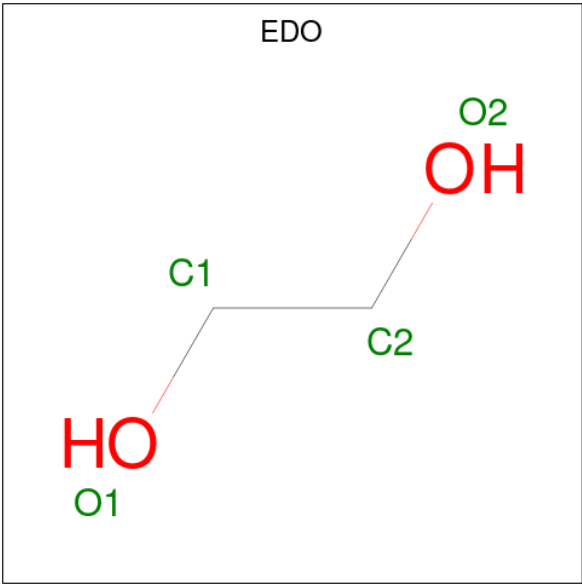
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	GLY	-	expression tag	UNP A0A2Y9UCL1
AAA	0	HIS	-	expression tag	UNP A0A2Y9UCL1
AAA	154	ILE	MET	variant	UNP A0A2Y9UCL1
AAA	283	THR	ALA	variant	UNP A0A2Y9UCL1
BBB	-1	GLY	-	expression tag	UNP A0A2Y9UCL1
BBB	0	HIS	-	expression tag	UNP A0A2Y9UCL1
BBB	154	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 (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



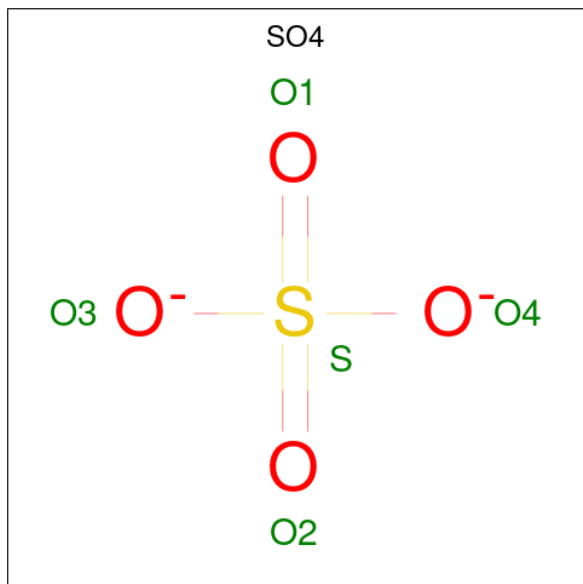
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	BBB	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	CCC	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	DDD	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



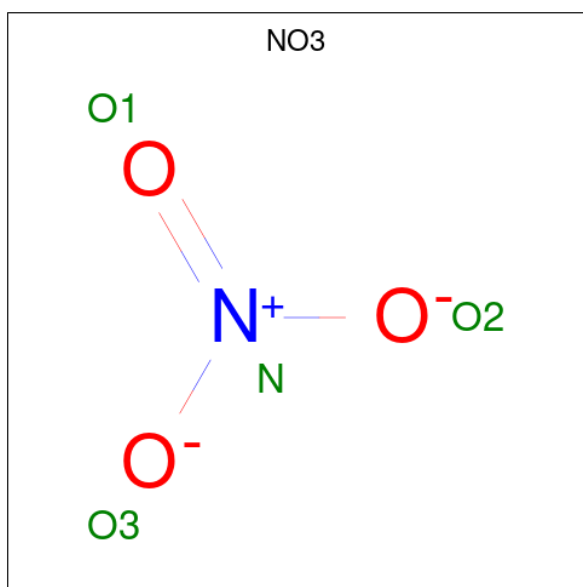
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	DDD	1	Total C O 4 2 2	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



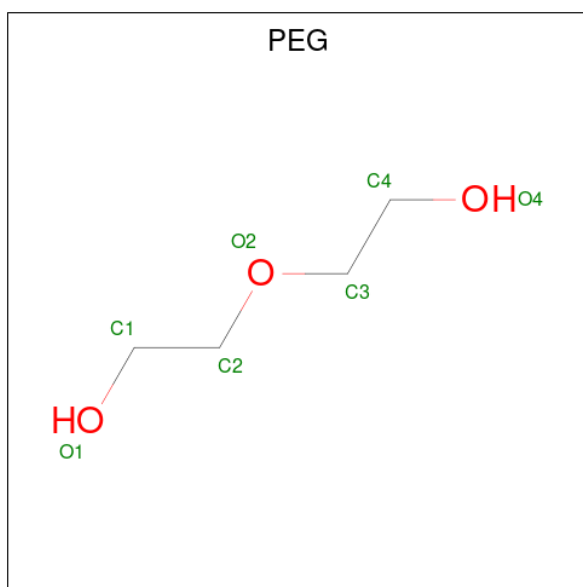
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total O S 5 4 1	0	0
4	AAA	1	Total O S 5 4 1	0	0

- Molecule 5 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

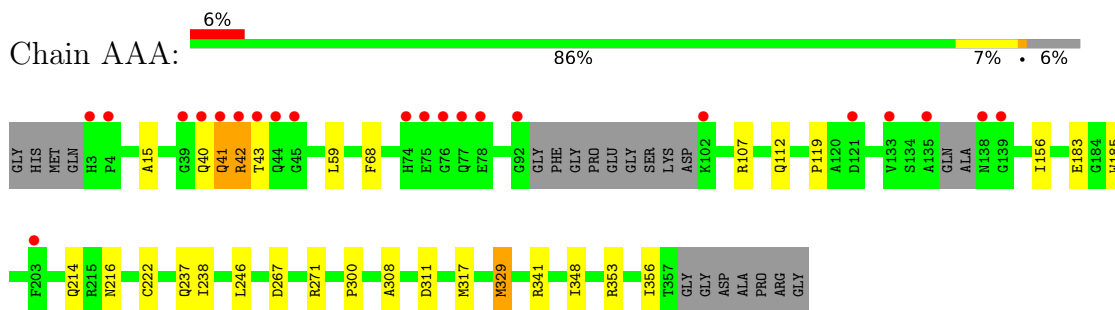
- Molecule 8 is water.

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

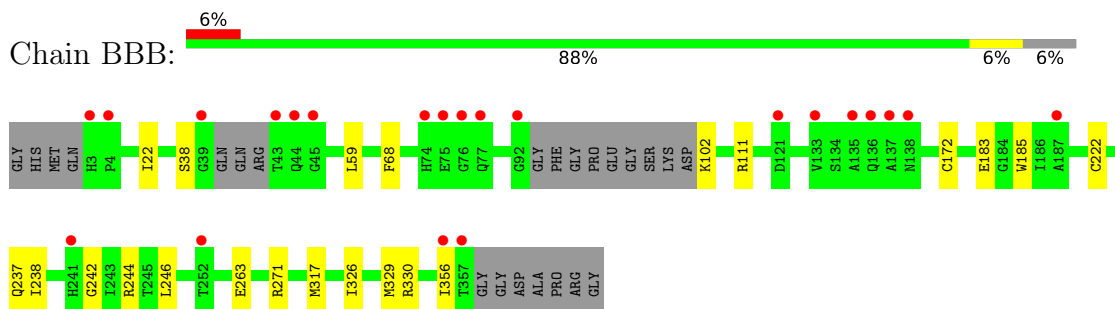
3 Residue-property plots [i](#)

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.

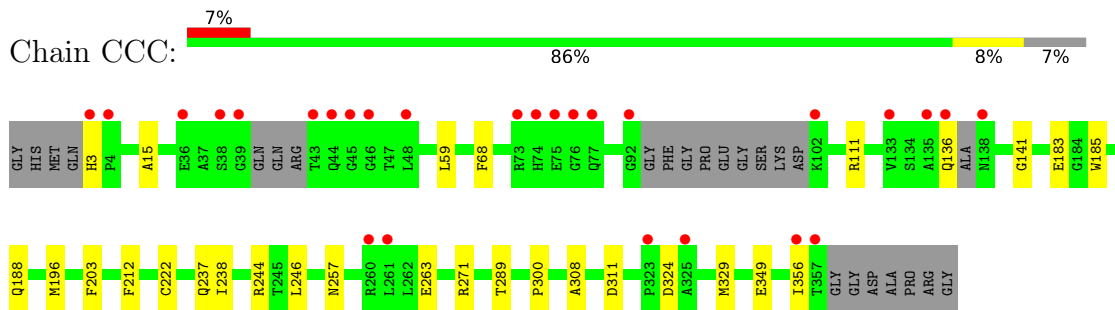
- Molecule 1: Monooxygenase



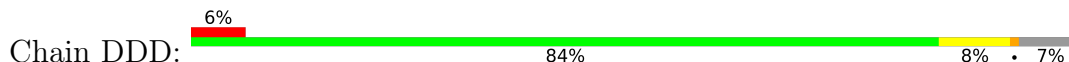
- Molecule 1: Monooxygenase

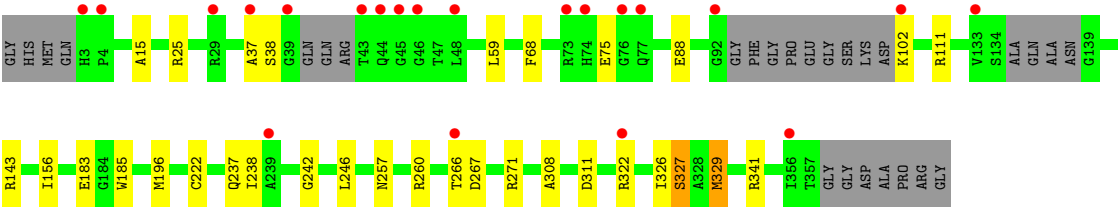


- Molecule 1: Monooxygenase



- Molecule 1: Monooxygenase





4 Data and refinement statistics

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 48.26 – 1.95	Depositor EDS
% Data completeness (in resolution range)	85.3 (48.26-1.95) 85.3 (48.26-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (3.35%)	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 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	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.*

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: PEG, SO4, EDO, FAD, NO3, CL

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	1.04	0/2703	1.34	3/3669 (0.1%)
1	BBB	1.04	0/2674	1.33	1/3631 (0.0%)
1	CCC	1.04	0/2680	1.32	1/3637 (0.0%)
1	DDD	1.03	0/2660	1.32	3/3610 (0.1%)
All	All	1.04	0/10717	1.33	8/14547 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	242	GLY	CA-C-O	-6.32	116.51	122.39
1	DDD	242	GLY	CA-C-O	-6.03	116.78	122.39
1	DDD	311	ASP	CA-CB-CG	5.75	118.36	112.60
1	AAA	311	ASP	CA-CB-CG	5.16	117.76	112.60
1	CCC	311	ASP	CA-CB-CG	5.15	117.75	112.60
1	AAA	119	PRO	CA-C-N	5.11	127.13	120.28
1	AAA	119	PRO	C-N-CA	5.11	127.13	120.28
1	DDD	37	ALA	CA-C-O	-5.00	116.10	121.56

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	21	0
1	BBB	2609	0	2575	10	0
1	CCC	2613	0	2579	17	0
1	DDD	2596	0	2567	18	0
2	AAA	53	0	31	0	0
2	BBB	53	0	31	0	0
2	CCC	53	0	31	0	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	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (66) 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:AAA:317[B]:MET:HE1	8:AAA:630:HOH:O	1.86	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
1:AAA:341:ARG:HD3	8:AAA:576:HOH:O	1.97	0.65
1:BBB:22:ILE:HG23	1:BBB:317[B]:MET:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:41:GLN:HE21	1:AAA:42:ARG:HD3	1.62	0.64
1:CCC:3:HIS:CD2	8:CCC:636:HOH:O	2.51	0.63
1:DDD:322[A]:ARG:NH2	1:DDD:327:SER:OG	2.34	0.60
1:CCC:349[B]:GLU:HG2	8:CCC:536:HOH:O	2.02	0.60
1:AAA:353:ARG:NH1	8:AAA:504:HOH:O	2.32	0.59
1:BBB:22:ILE:CG2	1:BBB:317[B]:MET:HE2	2.33	0.59
1:DDD:25:ARG:NH1	8:DDD:503:HOH:O	2.36	0.58
1:BBB:330:ARG:NH2	8:BBB:504:HOH:O	2.38	0.57
1:AAA:317[B]:MET:CE	8:AAA:630:HOH:O	2.50	0.55
1:DDD:341:ARG:HD3	8:DDD:574:HOH:O	2.06	0.54
1:AAA:185:TRP:CH2	1:AAA:222:CYS:HB2	2.43	0.54
1:CCC:185:TRP:CH2	1:CCC:222:CYS:HB2	2.43	0.53
1:CCC:136:GLN:HG3	1:CCC:141:GLY:N	2.23	0.53
1:DDD:75:GLU:O	1:DDD:75:GLU:HG2	2.09	0.52
1:BBB:185:TRP:CH2	1:BBB:222:CYS:HB2	2.45	0.51
1:AAA:348:ILE:HG23	6:AAA:407:PEG:H31	1.93	0.51
1:BBB:183:GLU:OE1	1:BBB:271:ARG:NH1	2.43	0.50
1:DDD:185:TRP:CH2	1:DDD:222:CYS:HB2	2.46	0.50
1:DDD:183:GLU:OE1	1:DDD:271:ARG:NH1	2.43	0.50
1:AAA:41:GLN:NE2	1:AAA:112:GLN:OE1	2.45	0.49
1:AAA:40:GLN:O	1:AAA:43:THR:HG22	2.13	0.49
1:BBB:237:GLN:CB	1:BBB:246:LEU:HD13	2.42	0.48
1:CCC:324:ASP:OD1	8:CCC:501:HOH:O	2.20	0.48
1:CCC:349[B]:GLU:HA	1:CCC:349[B]:GLU:OE1	2.14	0.48
1:CCC:196:MET:HE1	1:CCC:257:ASN:HB2	1.96	0.47
1:DDD:59:LEU:HD13	1:DDD:68:PHE:HB2	1.97	0.47
1:DDD:238:ILE:HG13	1:DDD:246:LEU:HD22	1.97	0.47
1:CCC:238:ILE:HG13	1:CCC:246:LEU:HD22	1.98	0.46
1:AAA:107:ARG:NH2	8:AAA:505:HOH:O	2.36	0.46
1:AAA:216:ASN:HB3	8:AAA:691:HOH:O	2.15	0.46
1:BBB:244:ARG:NH2	1:BBB:263:GLU:O	2.49	0.46
1:BBB:238:ILE:HG13	1:BBB:246:LEU:HD22	1.97	0.46
1:DDD:237:GLN:CB	1:DDD:246:LEU:HD13	2.39	0.45
1:DDD:156:ILE:HG12	1:DDD:329:MET:HE1	1.99	0.45
1:DDD:196:MET:HE1	1:DDD:257:ASN:HB2	1.99	0.45
1:DDD:143:ARG:HB3	8:DDD:708:HOH:O	2.17	0.45
1:DDD:15:ALA:HB2	1:DDD:308:ALA:HB1	1.97	0.45
1:AAA:156:ILE:HG12	1:AAA:329:MET:HE1	1.98	0.44
1:CCC:289:THR:HG22	1:CCC:329:MET:HE2	2.00	0.44
1:DDD:260:ARG:NH1	8:DDD:519:HOH:O	2.50	0.44
1:AAA:238:ILE:HG13	1:AAA:246:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:42:ARG:N	1:AAA:42:ARG:HD2	2.33	0.44
1:AAA:183:GLU:OE1	1:AAA:271:ARG:NH2	2.51	0.43
1:AAA:15:ALA:HB2	1:AAA:308:ALA:HB1	1.99	0.43
1:CCC:183:GLU:OE1	1:CCC:271:ARG:NH2	2.52	0.43
1:AAA:267:ASP:OD2	8:AAA:501:HOH:O	2.21	0.42
1:BBB:59:LEU:HD13	1:BBB:68:PHE:HB2	2.01	0.42
1:CCC:244:ARG:NH2	1:CCC:263:GLU:O	2.53	0.41
1:CCC:59:LEU:HD13	1:CCC:68:PHE:HB2	2.02	0.41
1:DDD:322[A]:ARG:NH1	1:DDD:327:SER:OG	2.53	0.41
1:AAA:300:PRO:HA	7:AAA:408:CL:CL	2.58	0.41
1:CCC:203:PHE:HD1	1:CCC:212:PHE:CD1	2.39	0.41
1:CCC:300:PRO:HA	7:CCC:405:CL:CL	2.58	0.41
1:AAA:214[A]:GLN:HG2	8:AAA:683:HOH:O	2.21	0.41
1:CCC:15:ALA:HB2	1:CCC:308:ALA:HB1	2.01	0.40
1:DDD:322[A]:ARG:CZ	1:DDD:327:SER:OG	2.70	0.40
1:AAA:59:LEU:HD13	1:AAA:68:PHE:HB2	2.03	0.40
1:DDD:88:GLU:HB3	8:DDD:562:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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 ⓘ

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%)	57	54
1	BBB	262/273 (96%)	255 (97%)	7 (3%)	39	32
1	CCC	263/273 (96%)	261 (99%)	2 (1%)	73	74
1	DDD	261/273 (96%)	253 (97%)	8 (3%)	35	26
All	All	1052/1092 (96%)	1031 (98%)	21 (2%)	48	43

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	41	GLN
1	AAA	42	ARG
1	AAA	329	MET
1	AAA	356	ILE
1	BBB	38	SER
1	BBB	102	LYS
1	BBB	111	ARG
1	BBB	172	CYS
1	BBB	326	ILE
1	BBB	329	MET
1	BBB	356	ILE
1	CCC	111	ARG
1	CCC	356	ILE
1	DDD	38	SER
1	DDD	102	LYS
1	DDD	111	ARG
1	DDD	266	THR
1	DDD	267	ASP
1	DDD	326	ILE
1	DDD	327	SER
1	DDD	329	MET

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

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 ⓘ

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	$\# Z > 2$
6	PEG	DDD	403	-	6,6,6	0.32	0	5,5,5	0.18	0
5	NO3	AAA	406	-	1,3,3	0.16	0	0,3,3	-	-
3	EDO	CCC	404	-	3,3,3	0.36	0	2,2,2	0.09	0
5	NO3	BBB	403	-	1,3,3	0.33	0	0,3,3	-	-
4	SO4	AAA	403	-	4,4,4	0.31	0	6,6,6	0.39	0
6	PEG	AAA	407	-	6,6,6	0.56	0	5,5,5	0.35	0
2	FAD	DDD	401	-	58,58,58	0.76	2 (3%)	85,89,89	0.69	1 (1%)
3	EDO	CCC	402	-	3,3,3	0.20	0	2,2,2	0.08	0
3	EDO	AAA	405	-	3,3,3	0.11	0	2,2,2	0.14	0
3	EDO	DDD	402	-	3,3,3	0.09	0	2,2,2	0.25	0
3	EDO	BBB	402	-	3,3,3	0.44	0	2,2,2	0.38	0
3	EDO	AAA	402	-	3,3,3	0.24	0	2,2,2	0.12	0
2	FAD	CCC	401	-	58,58,58	0.71	0	85,89,89	0.75	2 (2%)
5	NO3	CCC	403	-	1,3,3	0.24	0	0,3,3	-	-
2	FAD	BBB	401	-	58,58,58	0.63	0	85,89,89	0.70	1 (1%)
2	FAD	AAA	401	-	58,58,58	0.57	0	85,89,89	0.70	0
4	SO4	AAA	404	-	4,4,4	0.26	0	6,6,6	0.08	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
6	PEG	DDD	403	-	-	1/4/4/4	-
3	EDO	CCC	404	-	-	0/1/1/1	-
6	PEG	AAA	407	-	-	0/4/4/4	-
2	FAD	DDD	401	-	-	0/34/50/50	0/6/6/6
3	EDO	CCC	402	-	-	0/1/1/1	-
3	EDO	AAA	405	-	-	1/1/1/1	-
3	EDO	DDD	402	-	-	0/1/1/1	-
3	EDO	BBB	402	-	-	0/1/1/1	-
3	EDO	AAA	402	-	-	0/1/1/1	-
2	FAD	CCC	401	-	-	0/34/50/50	0/6/6/6
2	FAD	BBB	401	-	-	3/34/50/50	0/6/6/6
2	FAD	AAA	401	-	-	2/34/50/50	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	401	FAD	C1'-C2'	-2.22	1.49	1.52
2	DDD	401	FAD	C2-N1	-2.15	1.31	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	401	FAD	C4-N3-C2	-2.16	121.80	125.64
2	DDD	401	FAD	C4-N3-C2	-2.13	121.85	125.64
2	CCC	401	FAD	O2P-P-O1P	2.11	122.28	112.44
2	BBB	401	FAD	O3'-C3'-C2'	2.06	113.62	108.93

There are no chirality outliers.

All (7) 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
2	BBB	401	FAD	O2'-C2'-C3'-O3'
2	BBB	401	FAD	O2'-C2'-C3'-C4'
3	AAA	405	EDO	O1-C1-C2-O2
2	BBB	401	FAD	C1'-C2'-C3'-O3'

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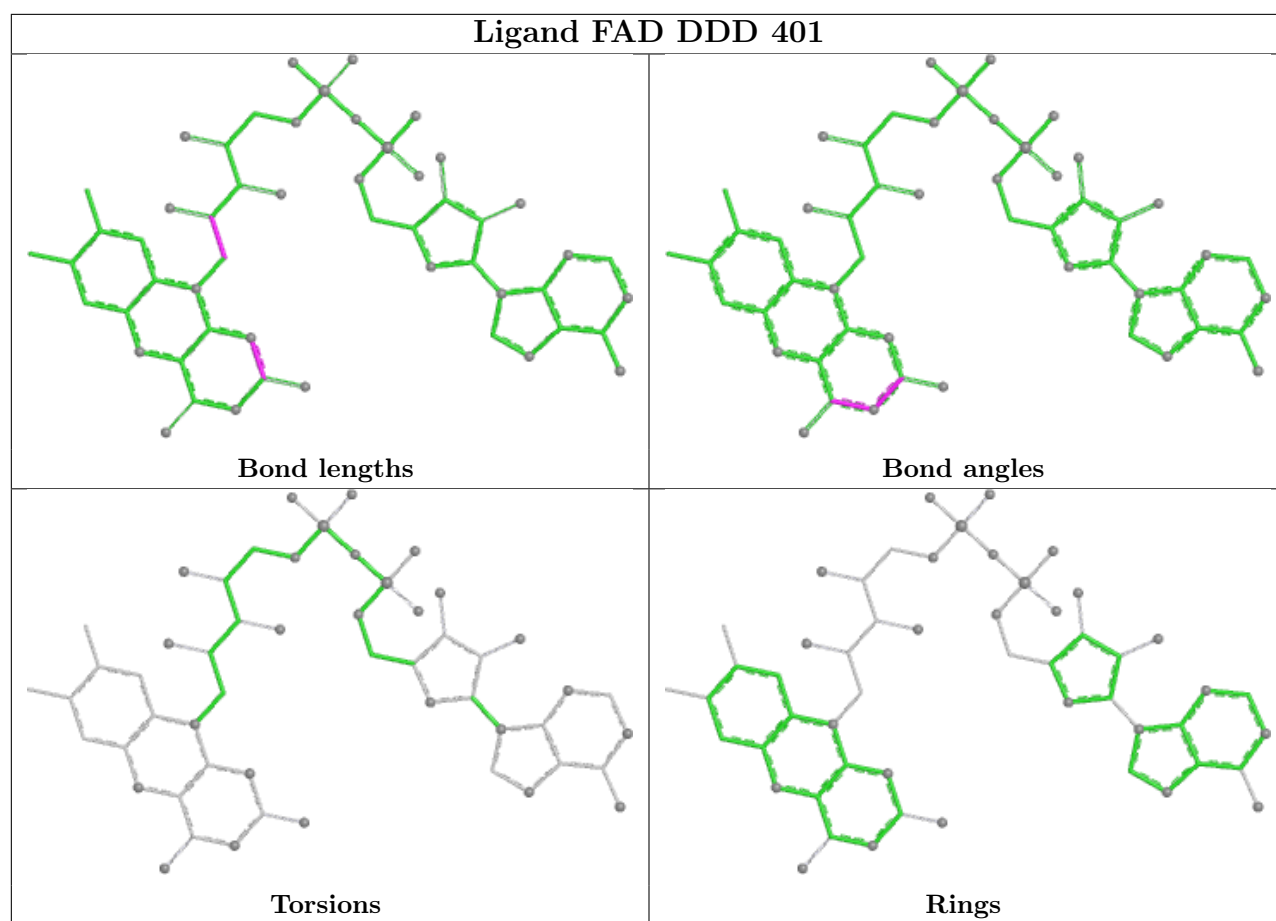
Mol	Chain	Res	Type	Atoms
2	AAA	401	FAD	O2'-C2'-C3'-C4'

There are no ring outliers.

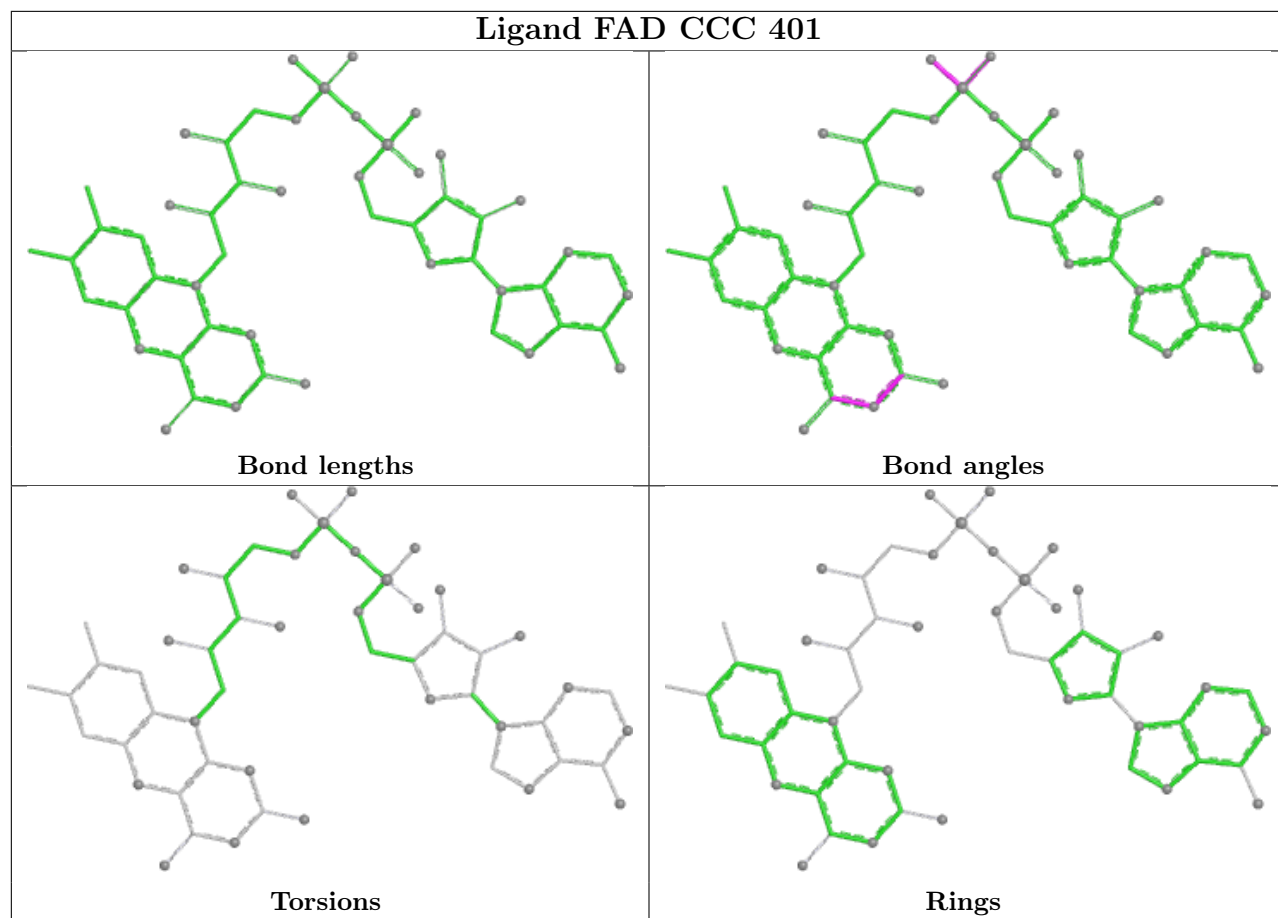
1 monomer is involved in 1 short contact:

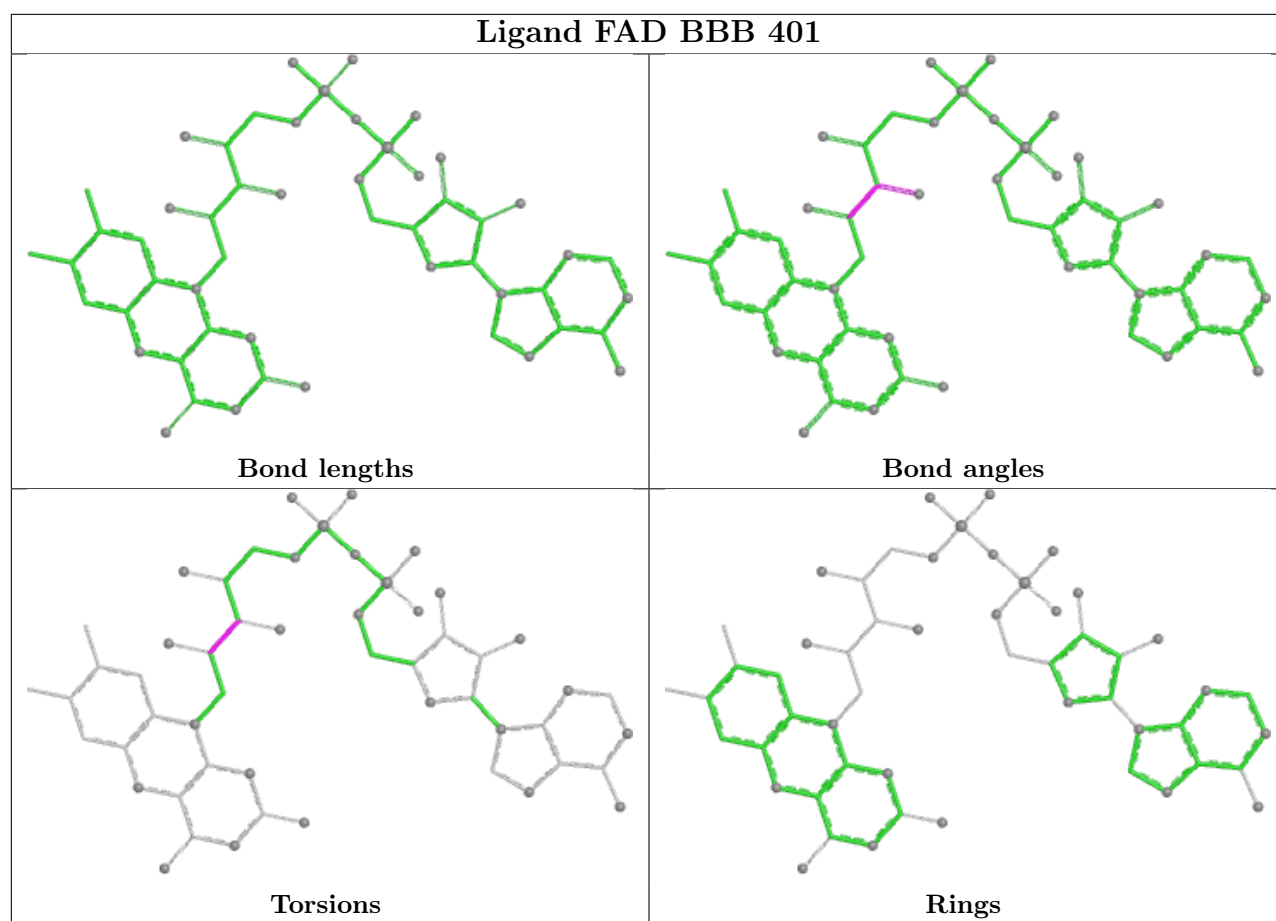
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AAA	407	PEG	1	0

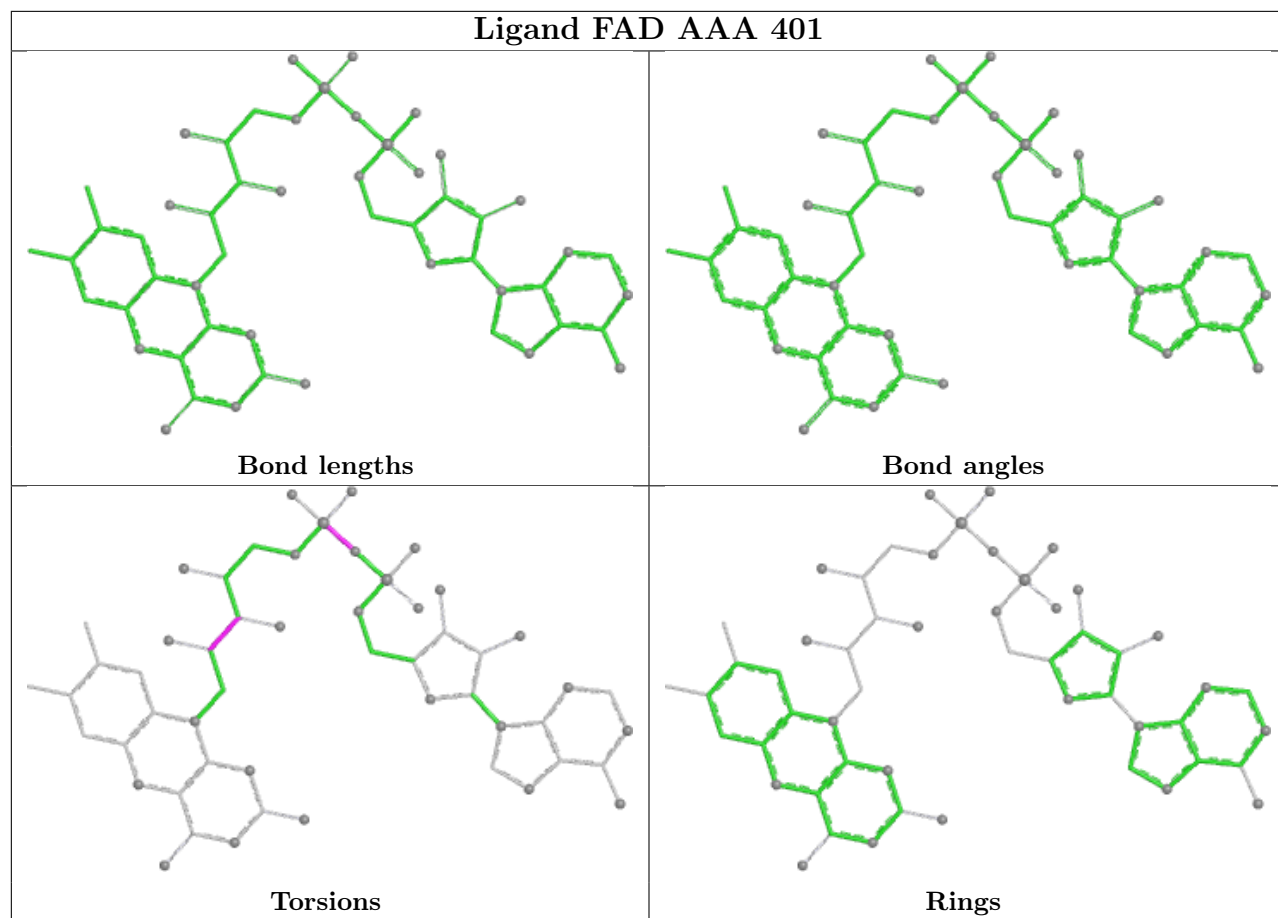
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 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, 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	AAA	344/366 (93%)	0.17	22 (6%) 25 29	13, 25, 61, 101	7 (2%)
1	BBB	343/366 (93%)	0.29	22 (6%) 25 29	13, 27, 58, 104	5 (1%)
1	CCC	342/366 (93%)	0.36	27 (7%) 18 21	14, 27, 61, 99	7 (2%)
1	DDD	339/366 (92%)	0.31	21 (6%) 26 31	15, 26, 53, 82	6 (1%)
All	All	1368/1464 (93%)	0.28	92 (6%) 24 27	13, 26, 59, 104	25 (1%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	39	GLY	5.8
1	BBB	43	THR	5.1
1	AAA	135	ALA	4.8
1	CCC	39	GLY	4.6
1	CCC	92	GLY	4.6
1	DDD	43	THR	4.3
1	BBB	76	GLY	4.0
1	CCC	102	LYS	4.0
1	BBB	137	ALA	4.0
1	CCC	43	THR	4.0
1	DDD	3	HIS	3.9
1	DDD	39	GLY	3.8
1	CCC	138	ASN	3.7
1	AAA	40	GLN	3.7
1	AAA	102	LYS	3.7
1	BBB	135	ALA	3.7
1	BBB	3	HIS	3.6
1	CCC	135	ALA	3.6
1	AAA	43	THR	3.6
1	AAA	92	GLY	3.5
1	AAA	76	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	CCC	3	HIS	3.4
1	AAA	44	GLN	3.4
1	CCC	73[A]	ARG	3.4
1	BBB	92	GLY	3.4
1	DDD	92	GLY	3.3
1	BBB	44	GLN	3.3
1	DDD	44	GLN	3.2
1	AAA	42	ARG	3.1
1	AAA	4	PRO	3.1
1	CCC	76	GLY	3.1
1	CCC	45	GLY	2.9
1	CCC	46	GLY	2.9
1	CCC	323	PRO	2.8
1	DDD	4	PRO	2.8
1	CCC	44	GLN	2.8
1	DDD	102	LYS	2.8
1	AAA	41	GLN	2.8
1	AAA	139	GLY	2.8
1	BBB	77	GLN	2.8
1	BBB	136	GLN	2.8
1	DDD	48	LEU	2.8
1	CCC	75	GLU	2.8
1	CCC	74	HIS	2.7
1	BBB	252	THR	2.7
1	AAA	39	GLY	2.7
1	AAA	78	GLU	2.7
1	DDD	46	GLY	2.7
1	BBB	121	ASP	2.6
1	CCC	38	SER	2.6
1	CCC	356	ILE	2.5
1	DDD	76	GLY	2.5
1	DDD	239	ALA	2.5
1	AAA	75	GLU	2.5
1	BBB	75	GLU	2.5
1	CCC	261	LEU	2.5
1	BBB	133	VAL	2.5
1	DDD	322[A]	ARG	2.5
1	AAA	3	HIS	2.5
1	CCC	77	GLN	2.5
1	CCC	260	ARG	2.4
1	BBB	138	ASN	2.4
1	AAA	77	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	CCC	4	PRO	2.4
1	AAA	133	VAL	2.4
1	DDD	74	HIS	2.4
1	DDD	29	ARG	2.3
1	AAA	138	ASN	2.3
1	BBB	74	HIS	2.3
1	BBB	356	ILE	2.2
1	CCC	357	THR	2.2
1	DDD	266	THR	2.2
1	CCC	48	LEU	2.2
1	AAA	45	GLY	2.2
1	AAA	121	ASP	2.2
1	DDD	73	ARG	2.2
1	CCC	136	GLN	2.2
1	AAA	203	PHE	2.2
1	DDD	356	ILE	2.2
1	BBB	4	PRO	2.2
1	DDD	133	VAL	2.1
1	BBB	45	GLY	2.1
1	BBB	357	THR	2.1
1	CCC	325	ALA	2.1
1	AAA	74	HIS	2.1
1	BBB	187	ALA	2.1
1	DDD	37	ALA	2.1
1	DDD	45	GLY	2.0
1	CCC	36	GLU	2.0
1	BBB	241	HIS	2.0
1	DDD	77	GLN	2.0
1	CCC	133	VAL	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 ⓘ

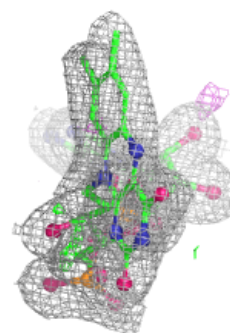
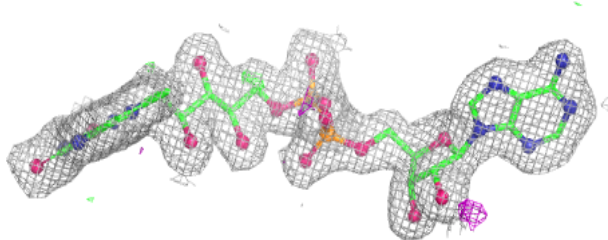
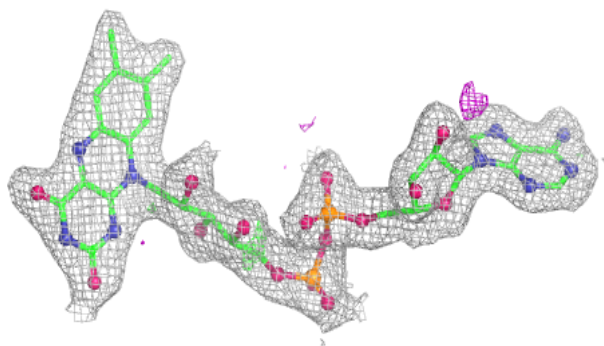
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PEG	AAA	407	7/7	0.80	0.16	34,40,47,47	0
6	PEG	DDD	403	7/7	0.88	0.12	33,35,39,42	0
4	SO4	AAA	404	5/5	0.89	0.12	51,65,69,72	0
3	EDO	CCC	404	4/4	0.90	0.10	36,37,41,43	0
5	NO3	AAA	406	4/4	0.91	0.18	36,47,49,59	0
5	NO3	BBB	403	4/4	0.91	0.14	44,47,47,53	0
3	EDO	AAA	405	4/4	0.92	0.10	36,36,36,42	0
4	SO4	AAA	403	5/5	0.93	0.09	33,37,43,46	0
5	NO3	CCC	403	4/4	0.94	0.10	42,45,45,46	0
3	EDO	BBB	402	4/4	0.96	0.06	24,24,27,28	0
3	EDO	DDD	402	4/4	0.97	0.06	24,27,27,28	0
3	EDO	CCC	402	4/4	0.97	0.05	18,20,21,21	0
2	FAD	CCC	401	53/53	0.98	0.05	14,20,24,29	0
2	FAD	DDD	401	53/53	0.98	0.05	14,18,23,27	0
3	EDO	AAA	402	4/4	0.98	0.04	18,19,19,20	0
2	FAD	AAA	401	53/53	0.98	0.05	13,16,25,34	0
2	FAD	BBB	401	53/53	0.98	0.05	13,17,24,27	0
7	CL	AAA	408	1/1	0.99	0.03	22,22,22,22	0
7	CL	BBB	404	1/1	0.99	0.03	21,21,21,21	0
7	CL	CCC	405	1/1	0.99	0.03	21,21,21,21	0
7	CL	DDD	404	1/1	0.99	0.04	21,21,21,21	0

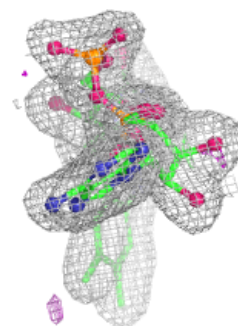
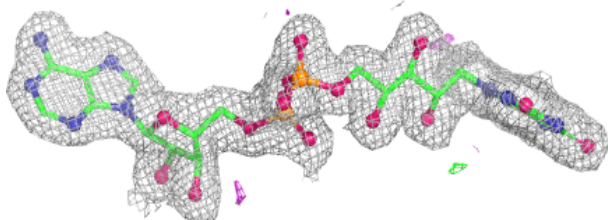
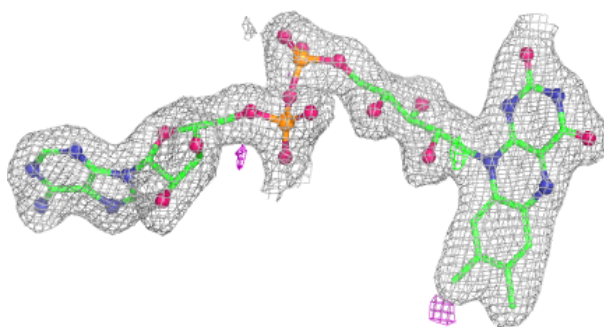
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

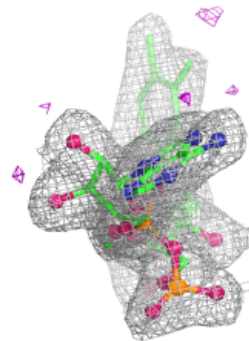
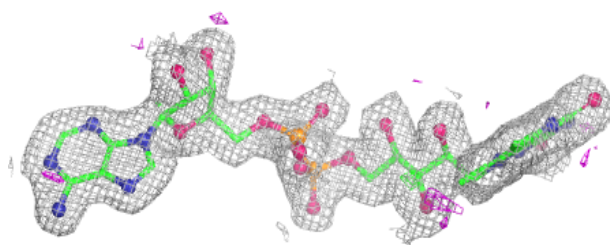
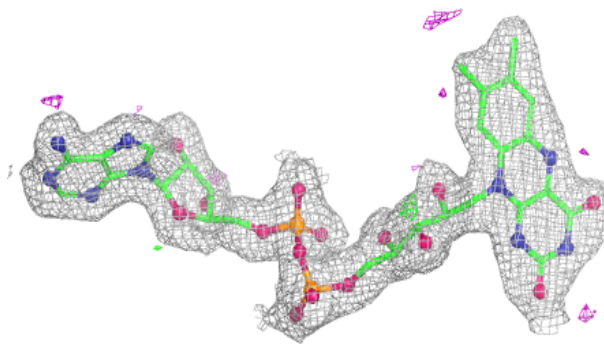
**Electron density around FAD DDD 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

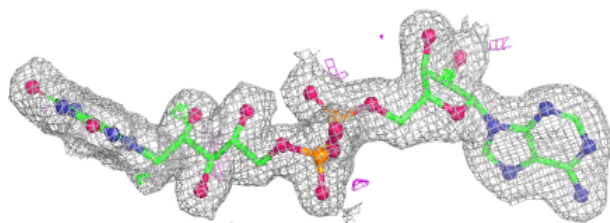
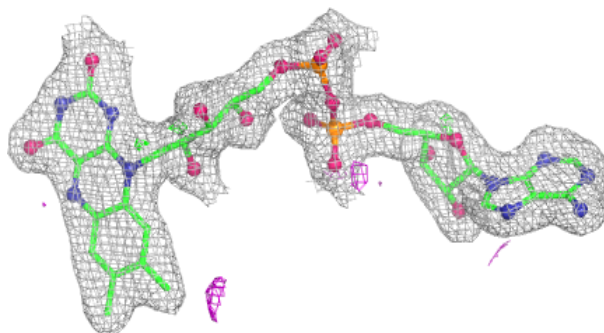


Electron density around FAD AAA 401:

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

**Electron density around FAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.