Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:52 PM UTC

PDB ID	:	7V0B / pdb_00007v0b
Title	:	Crystal structure of halogenase CtcP from Kitasatospora aureofaciens in complex with FAD
Authors	:	Hou, C.; Tsodikov, O.V.
Deposited on	:	2022-05-10
Resolution	:	2.15 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:

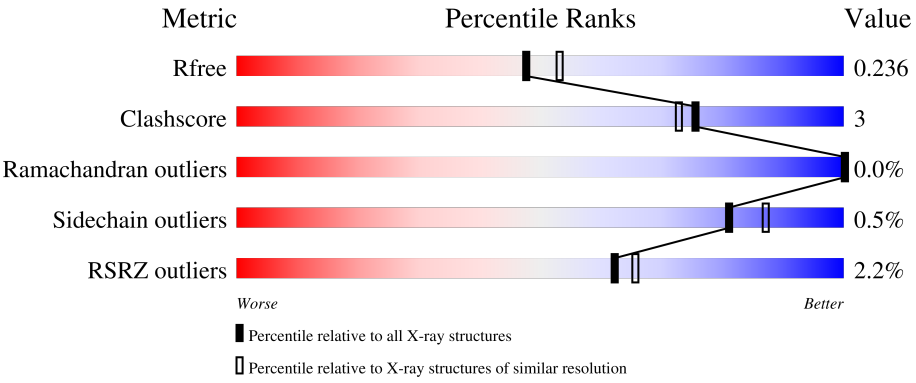
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	A	558	91% 6% ·
1	B	558	2% 87% 7% 5%
1	C	558	88% 7% ·
1	D	558	5% 87% 7% 6%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18178 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.

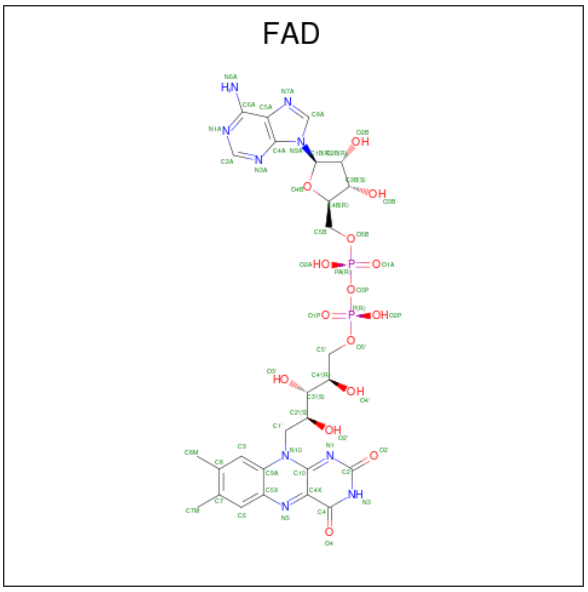
- Molecule 1 is a protein called Tetracycline 7-halogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4293	2699	776	798	20			
1	B	528	Total	C	N	O	S	0	0	0
			4209	2651	759	780	19			
1	C	535	Total	C	N	O	S	0	0	0
			4264	2682	769	794	19			
1	D	527	Total	C	N	O	S	0	0	0
			4207	2649	758	781	19			

There are 12 discrepancies between the modelled and reference sequences:

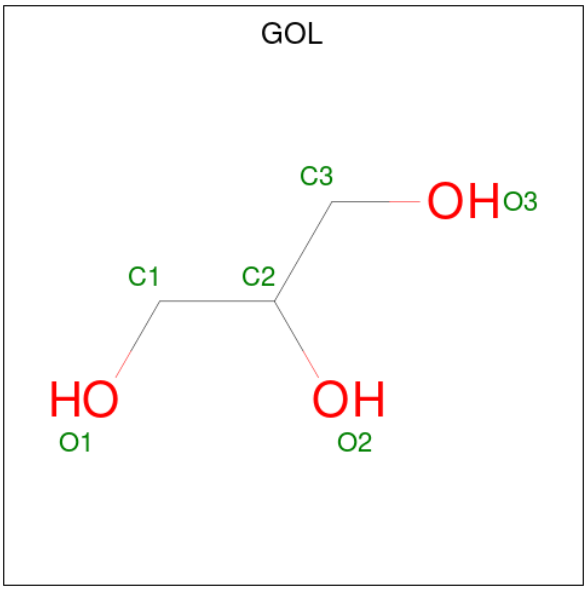
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A1E7MYN1
A	-1	PRO	-	expression tag	UNP A0A1E7MYN1
A	0	HIS	-	expression tag	UNP A0A1E7MYN1
B	-2	GLY	-	expression tag	UNP A0A1E7MYN1
B	-1	PRO	-	expression tag	UNP A0A1E7MYN1
B	0	HIS	-	expression tag	UNP A0A1E7MYN1
C	-2	GLY	-	expression tag	UNP A0A1E7MYN1
C	-1	PRO	-	expression tag	UNP A0A1E7MYN1
C	0	HIS	-	expression tag	UNP A0A1E7MYN1
D	-2	GLY	-	expression tag	UNP A0A1E7MYN1
D	-1	PRO	-	expression tag	UNP A0A1E7MYN1
D	0	HIS	-	expression tag	UNP A0A1E7MYN1

- 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	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

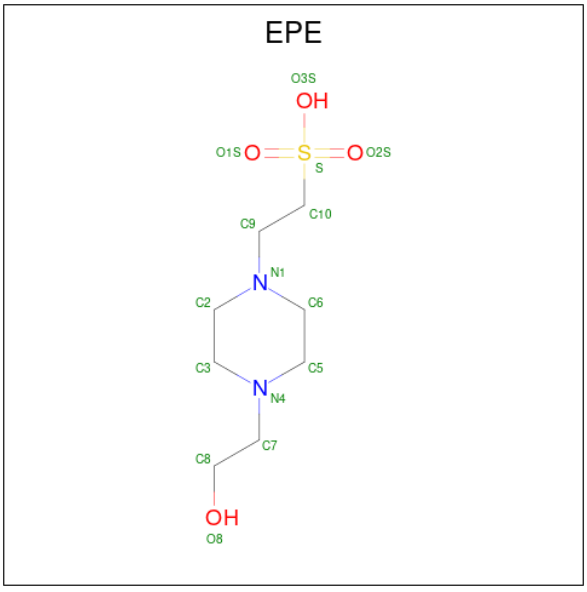


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O S 15 8 2 4 1	0	0
5	C	1	Total C N O S 13 7 2 3 1	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Na 1 1	0	0

- Molecule 7 is water.

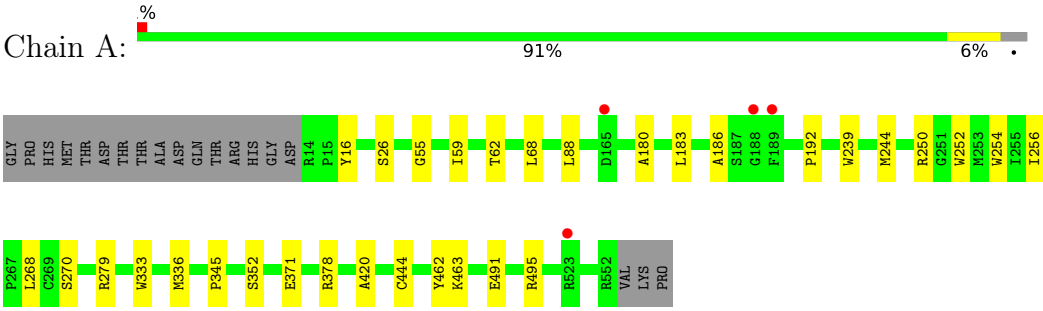
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	339	Total O 339 339	0	0
7	B	282	Total O 282 282	0	0
7	C	215	Total O 215 215	0	0
7	D	106	Total O 106 106	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

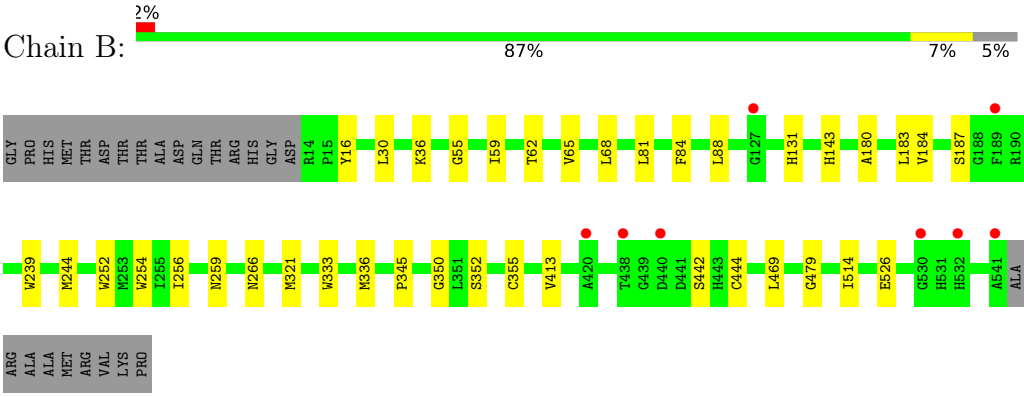
• Molecule 1: Tetracycline 7-halogenase

Chain A:



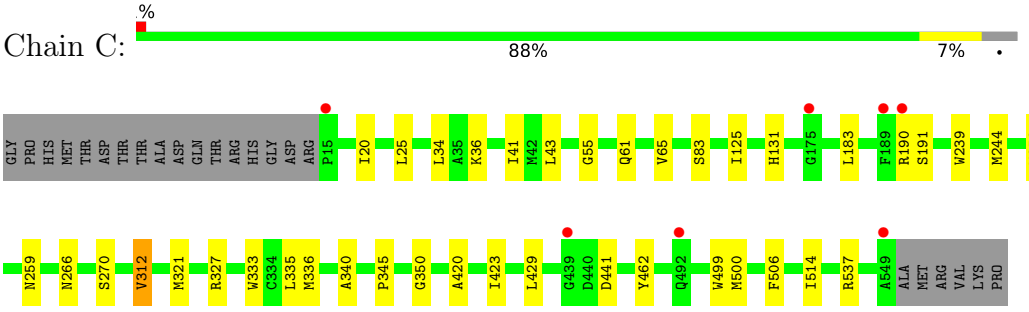
• Molecule 1: Tetracycline 7-halogenase

Chain B:



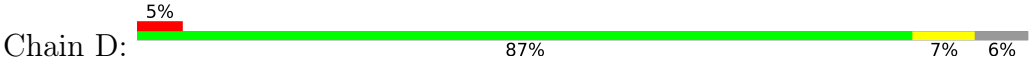
• Molecule 1: Tetracycline 7-halogenase

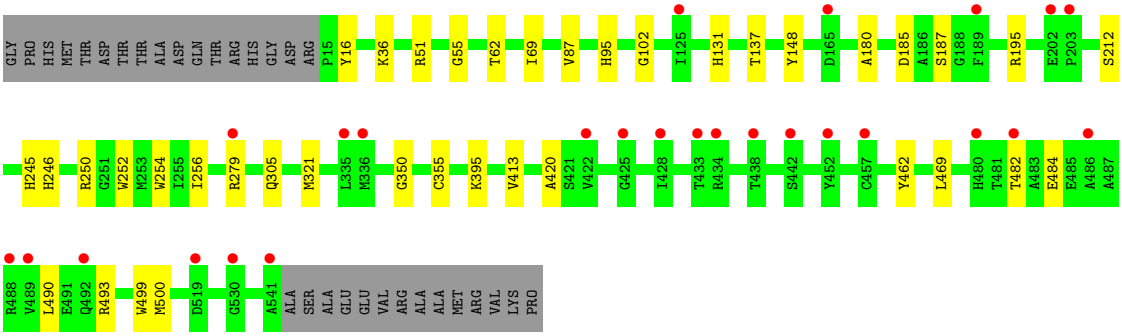
Chain C:



• Molecule 1: Tetracycline 7-halogenase

Chain D:




GLY PRO HIS MET THR ASP THR THR ALA ASP GLN THR ARG HIS GLY ASP ARG P15 Y16 K36 R51 G55 T62 I69 V87 H95 G102 I125 H131 T137 Y148 D165 A180 D185 A186 S187 G188 F189 R195 E202 P203 S212
H245 H246 R250 G251 W252 M253 W254 I255 I256 R279 Q305 M321 L335 M336 G350 C355 K395 V413 A420 S421 V422 G425 I428 T433 R434 T438 S442 Y452 C457 Y462 L469 H480 T481 T482 A483 E484 E485 A486 A487
R488 V489 L490 E491 Q492 R493 W499 M500 D519 G530 A541 ALA SER ALA GLU GLU VAL ARG ALA ALA MET ARG VAL LYS PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.76Å 103.58Å 179.22Å 90.00° 95.40° 90.00°	Depositor
Resolution (Å)	35.00 – 2.15 35.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.9 (35.00-2.15) 96.9 (35.00-2.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.188 , 0.233 0.194 , 0.236	Depositor DCC
R_{free} test set	6222 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.4	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	18178	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, EPE, CL, NA, GOL

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	0.98	0/4409	1.34	0/5990
1	B	0.98	0/4325	1.36	2/5878 (0.0%)
1	C	0.99	0/4380	1.37	3/5951 (0.1%)
1	D	0.99	0/4323	1.38	0/5874
All	All	0.98	0/17437	1.36	5/23693 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	312	VAL	N-CA-C	-5.29	107.97	113.10
1	B	526	GLU	CA-C-N	5.21	127.25	120.28
1	B	526	GLU	C-N-CA	5.21	127.25	120.28
1	C	423	ILE	CA-C-N	5.02	125.56	119.98
1	C	423	ILE	C-N-CA	5.02	125.56	119.98

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4293	0	4093	27	0
1	B	4209	0	4010	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4264	0	4065	26	0
1	D	4207	0	4011	23	0
2	A	53	0	31	4	0
2	B	53	0	31	4	0
2	C	53	0	31	5	0
2	D	53	0	31	3	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	15	0	18	0	0
5	C	13	0	13	1	0
6	C	1	0	0	0	0
7	A	339	0	0	3	0
7	B	282	0	0	1	0
7	C	215	0	0	2	0
7	D	106	0	0	2	0
All	All	18178	0	16358	102	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 (102) 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:55:GLY:HA2	2:C:601:FAD:C4X	2.13	0.77
1:A:55:GLY:HA2	2:A:601:FAD:C4X	2.16	0.75
1:A:62:THR:HG21	7:A:835:HOH:O	1.87	0.74
1:B:55:GLY:HA2	2:B:601:FAD:C4X	2.17	0.74
1:D:62:THR:HG21	7:D:712:HOH:O	1.94	0.68
1:A:239:TRP:HB3	1:A:244:MET:HE3	1.75	0.68
1:C:345:PRO:HG3	2:C:601:FAD:C6	2.26	0.65
1:C:239:TRP:HB3	1:C:244:MET:HE3	1.80	0.63
1:A:336:MET:HG3	7:A:939:HOH:O	1.98	0.63
1:D:55:GLY:HA2	2:D:601:FAD:C4X	2.29	0.62
1:A:491:GLU:OE2	1:A:495:ARG:NH1	2.33	0.61
1:C:239:TRP:CE3	1:C:244:MET:HE1	2.37	0.60
1:A:239:TRP:CE3	1:A:244:MET:HE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:GLY:HA3	2:B:601:FAD:H1'2	1.85	0.58
1:A:62:THR:HG22	1:A:352:SER:CA	2.34	0.57
1:B:62:THR:HG22	1:B:352:SER:CA	2.34	0.57
1:A:345:PRO:HG3	2:A:601:FAD:C6	2.36	0.55
1:B:30:LEU:HD22	1:B:336:MET:HE1	1.89	0.55
1:A:420:ALA:HB2	1:A:462:TYR:CE1	2.42	0.55
1:C:420:ALA:HB2	1:C:462:TYR:CE1	2.41	0.55
1:A:259:ASN:HB3	1:A:266:ASN:O	2.07	0.54
1:D:55:GLY:HA2	2:D:601:FAD:C10	2.37	0.54
1:B:239:TRP:CE3	1:B:244:MET:HE1	2.43	0.53
1:B:345:PRO:HG3	2:B:601:FAD:C6	2.39	0.53
1:B:413:VAL:HG22	1:B:469:LEU:HD11	1.92	0.52
1:B:62:THR:HG21	7:B:734:HOH:O	2.09	0.52
1:A:252:TRP:CZ3	1:A:254:TRP:HB3	2.45	0.51
1:D:16:TYR:O	1:D:180:ALA:HA	2.12	0.49
1:D:499:TRP:CZ2	1:D:500:MET:HE2	2.48	0.49
1:B:68:LEU:HD11	1:B:444:CYS:SG	2.52	0.49
1:A:62:THR:HG22	1:A:352:SER:HA	1.94	0.48
1:A:68:LEU:HD11	1:A:444:CYS:SG	2.53	0.48
1:A:183:LEU:O	1:A:333:TRP:HA	2.13	0.48
1:B:184:VAL:CG1	1:B:336:MET:HE2	2.44	0.48
1:D:185:ASP:OD1	1:D:187:SER:OG	2.28	0.47
1:A:250:ARG:HG3	1:A:279:ARG:CD	2.44	0.47
1:B:62:THR:HG22	1:B:352:SER:HA	1.96	0.47
1:C:183:LEU:O	1:C:333:TRP:HA	2.15	0.47
1:C:499:TRP:CZ2	1:C:500:MET:HE2	2.50	0.47
1:C:321:MET:HE1	2:C:601:FAD:HM72	1.95	0.47
1:D:69:ILE:HD11	1:D:355:CYS:O	2.15	0.47
1:D:420:ALA:HB2	1:D:462:TYR:CZ	2.50	0.47
1:A:26:SER:OG	1:A:186:ALA:HB1	2.15	0.46
1:B:59:ILE:HG12	1:B:62:THR:HG23	1.97	0.46
1:D:252:TRP:CZ3	1:D:254:TRP:HB3	2.50	0.46
1:B:187:SER:OG	1:B:191:SER:HA	2.15	0.46
1:B:259:ASN:HB3	1:B:266:ASN:O	2.16	0.45
1:D:490:LEU:O	1:D:493:ARG:HB3	2.16	0.45
1:A:250:ARG:HG3	1:A:279:ARG:HD2	1.99	0.45
1:C:506:PHE:CZ	1:C:514:ILE:HG21	2.51	0.45
1:B:212:SER:HB2	1:B:321:MET:SD	2.56	0.45
1:B:321:MET:HE1	2:B:601:FAD:HM72	1.99	0.45
1:B:479:GLY:O	1:C:537:ARG:NH2	2.49	0.45
1:B:252:TRP:CZ3	1:B:254:TRP:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ILE:HB	1:C:43:LEU:HD23	1.99	0.45
1:C:252:TRP:CZ3	1:C:254:TRP:HB3	2.52	0.45
1:C:336:MET:HE3	7:C:852:HOH:O	2.16	0.44
1:A:16:TYR:O	1:A:180:ALA:HA	2.18	0.44
1:A:371:GLU:OE2	1:A:378:ARG:NH2	2.46	0.44
1:C:55:GLY:HA2	2:C:601:FAD:C10	2.48	0.44
1:B:84:PHE:CZ	1:B:88:LEU:HD11	2.53	0.43
1:C:335:LEU:HD23	1:C:340:ALA:HA	2.01	0.43
1:C:131:HIS:CG	1:C:256:ILE:HG23	2.53	0.43
1:D:246:HIS:HE1	1:D:305:GLN:OE1	2.01	0.43
1:A:192:PRO:HG3	2:A:601:FAD:N6A	2.34	0.43
1:A:420:ALA:HB2	1:A:462:TYR:CZ	2.53	0.43
1:B:131:HIS:CG	1:B:256:ILE:HG23	2.53	0.43
1:A:256:ILE:HB	1:A:270:SER:HB3	2.01	0.43
1:D:250:ARG:HG3	1:D:279:ARG:HD2	2.00	0.43
1:C:125:ILE:HG13	1:C:429:LEU:HD13	1.99	0.43
1:D:102:GLY:O	1:D:245:HIS:HD2	2.01	0.43
1:D:195:ARG:NH2	7:D:701:HOH:O	2.42	0.43
1:B:16:TYR:O	1:B:180:ALA:HA	2.18	0.42
1:C:327:ARG:HD2	7:C:762:HOH:O	2.18	0.42
1:A:62:THR:HG22	1:A:352:SER:N	2.34	0.42
1:C:256:ILE:HB	1:C:270:SER:HB3	2.01	0.42
1:D:131:HIS:CG	1:D:256:ILE:HG23	2.55	0.42
1:B:184:VAL:HG11	1:B:336:MET:CE	2.49	0.42
1:D:420:ALA:HB2	1:D:462:TYR:CE1	2.55	0.42
1:B:65:VAL:HG12	1:B:355:CYS:HB3	2.01	0.42
1:A:268:LEU:HD11	1:B:143:HIS:CE1	2.55	0.42
1:D:87:VAL:CG1	1:D:95:HIS:CD2	3.03	0.42
1:D:482:THR:HG22	1:D:484:GLU:OE1	2.20	0.42
1:B:131:HIS:CD2	1:B:256:ILE:HG23	2.56	0.41
1:C:34:LEU:HB3	1:C:41:ILE:HD11	2.01	0.41
1:D:350:GLY:HA3	2:D:601:FAD:H1'2	2.01	0.41
1:A:59:ILE:HG12	1:A:62:THR:HG23	2.03	0.41
1:C:350:GLY:HA3	2:C:601:FAD:H1'2	2.03	0.41
1:D:87:VAL:HG12	1:D:95:HIS:CD2	2.56	0.41
1:D:36:LYS:HG3	1:D:148:TYR:CE1	2.55	0.41
1:A:55:GLY:HA2	2:A:601:FAD:C10	2.48	0.41
1:B:183:LEU:O	1:B:333:TRP:HA	2.20	0.41
1:C:259:ASN:HB3	1:C:266:ASN:O	2.21	0.41
1:A:463:LYS:NZ	7:A:710:HOH:O	2.51	0.41
1:B:184:VAL:HG11	1:B:336:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ARG:O	1:C:191:SER:C	2.63	0.41
1:D:212:SER:HB2	1:D:321:MET:SD	2.61	0.41
1:B:514:ILE:N	1:B:514:ILE:HD12	2.36	0.40
1:C:441:ASP:OD2	5:C:603:EPE:H32	2.21	0.40
1:C:61:GLN:O	1:C:65:VAL:HG23	2.20	0.40
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.95	0.40
1:D:413:VAL:HG22	1:D:469:LEU:HD11	2.03	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	537/558 (96%)	524 (98%)	13 (2%)	0	100	100
1	B	526/558 (94%)	511 (97%)	14 (3%)	1 (0%)	43	44
1	C	533/558 (96%)	520 (98%)	13 (2%)	0	100	100
1	D	525/558 (94%)	511 (97%)	14 (3%)	0	100	100
All	All	2121/2232 (95%)	2066 (97%)	54 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	442	SER

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	A	453/470 (96%)	452 (100%)	1 (0%)	87 92
1	B	445/470 (95%)	443 (100%)	2 (0%)	84 89
1	C	451/470 (96%)	448 (99%)	3 (1%)	76 82
1	D	446/470 (95%)	443 (99%)	3 (1%)	76 82
All	All	1795/1880 (96%)	1786 (100%)	9 (0%)	81 87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	B	36	LYS
1	B	81	LEU
1	C	36	LYS
1	C	83	SER
1	C	312	VAL
1	D	51	ARG
1	D	137	THR
1	D	395	LYS

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

Mol	Chain	Res	Type
1	A	100	ASN
1	A	119	GLN
1	A	338	HIS
1	A	359	ASN
1	A	406	HIS
1	B	135	GLN
1	B	406	HIS
1	B	443	HIS
1	B	445	GLN
1	C	128	ASN
1	C	135	GLN
1	C	160	ASN
1	C	240	ASN
1	C	532	HIS
1	D	245	HIS
1	D	246	HIS

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 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
3	GOL	A	602	-	5,5,5	0.12	0	5,5,5	0.29	0
5	EPE	B	603	-	15,15,15	0.60	1 (6%)	19,20,20	0.72	1 (5%)
3	GOL	C	602	-	5,5,5	0.12	0	5,5,5	0.29	0
2	FAD	B	601	-	58,58,58	0.60	0	85,89,89	0.66	1 (1%)
2	FAD	C	601	-	58,58,58	0.63	1 (1%)	85,89,89	0.66	2 (2%)
2	FAD	D	601	-	58,58,58	0.57	0	85,89,89	0.63	1 (1%)
5	EPE	C	603	-	13,13,15	0.67	1 (7%)	17,18,20	0.77	0
2	FAD	A	601	-	58,58,58	0.59	0	85,89,89	0.71	1 (1%)
3	GOL	B	602	-	5,5,5	0.07	0	5,5,5	0.23	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
3	GOL	A	602	-	-	0/4/4/4	-
5	EPE	B	603	-	-	1/9/19/19	0/1/1/1
3	GOL	C	602	-	-	0/4/4/4	-
2	FAD	B	601	-	-	2/34/50/50	0/6/6/6
2	FAD	C	601	-	-	11/34/50/50	0/6/6/6
2	FAD	D	601	-	-	0/34/50/50	0/6/6/6
5	EPE	C	603	-	-	2/6/16/19	0/1/1/1
2	FAD	A	601	-	-	13/34/50/50	0/6/6/6
3	GOL	B	602	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	P-O3P	2.20	1.61	1.59
5	B	603	EPE	O3S-S	2.14	1.55	1.47
5	C	603	EPE	O3S-S	2.10	1.55	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	603	EPE	O3S-S-C10	-2.47	101.17	106.00
2	A	601	FAD	C1'-C2'-C3'	2.20	115.63	109.66
2	C	601	FAD	C1'-C2'-C3'	2.14	115.46	109.66
2	C	601	FAD	C4-N3-C2	-2.12	121.88	125.64
2	B	601	FAD	C1'-C2'-C3'	2.11	115.39	109.66
2	D	601	FAD	C4-N3-C2	-2.07	121.97	125.64

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O2A
2	A	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	C3'-C4'-C5'-O5'
2	A	601	FAD	O4'-C4'-C5'-O5'
2	A	601	FAD	C5'-O5'-P-O1P
2	A	601	FAD	C5'-O5'-P-O2P
2	A	601	FAD	C5'-O5'-P-O3P
2	A	601	FAD	PA-O3P-P-O5'
2	B	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	C	601	FAD	C5B-O5B-PA-O2A
2	C	601	FAD	C5B-O5B-PA-O3P
2	C	601	FAD	C3'-C4'-C5'-O5'
2	C	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	C5'-O5'-P-O2P
2	C	601	FAD	C5'-O5'-P-O3P
2	C	601	FAD	PA-O3P-P-O5'
5	C	603	EPE	C10-C9-N1-C6
2	C	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	C3B-C4B-C5B-O5B
5	C	603	EPE	C10-C9-N1-C2
5	B	603	EPE	N4-C7-C8-O8
2	A	601	FAD	C5B-O5B-PA-O1A
2	C	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	C1'-C2'-C3'-O3'
2	B	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	P-O3P-PA-O2A

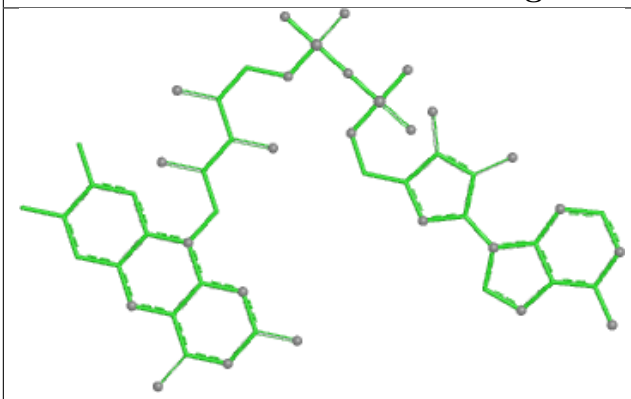
There are no ring outliers.

5 monomers are involved in 17 short contacts:

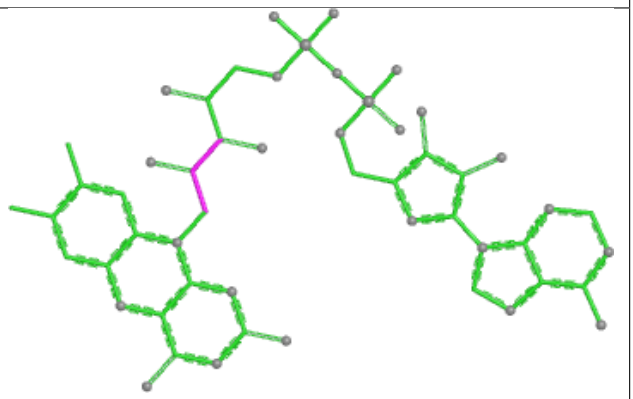
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FAD	4	0
2	C	601	FAD	5	0
2	D	601	FAD	3	0
5	C	603	EPE	1	0
2	A	601	FAD	4	0

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.

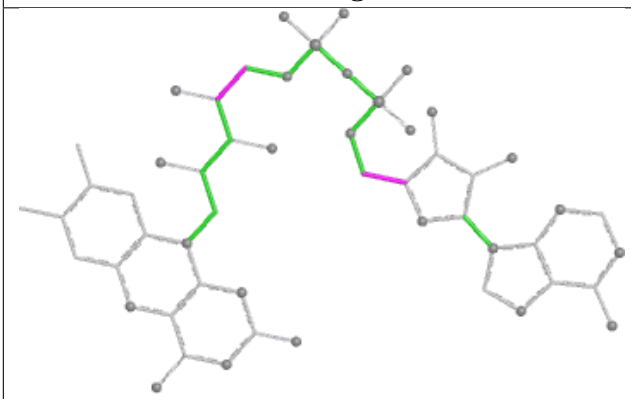
Ligand FAD B 601



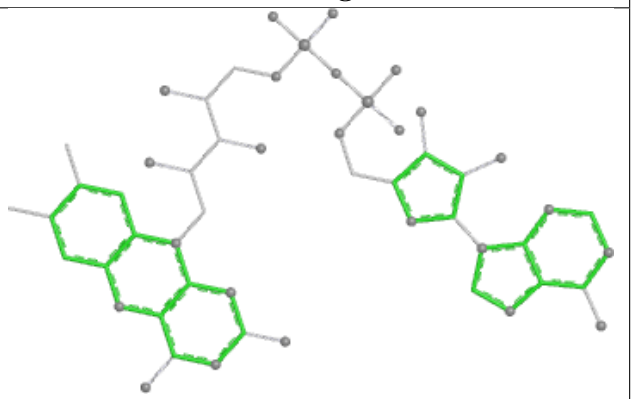
Bond lengths



Bond angles

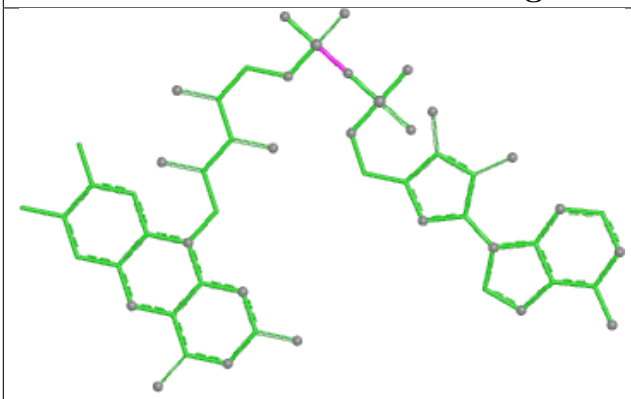


Torsions

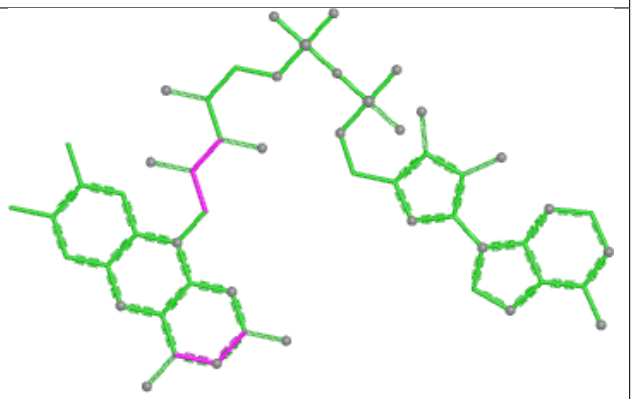


Rings

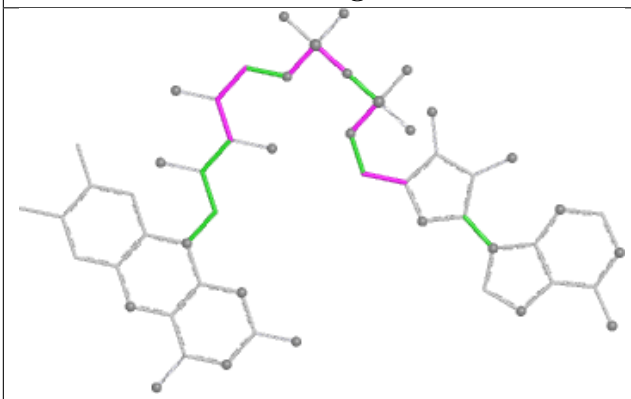
Ligand FAD C 601



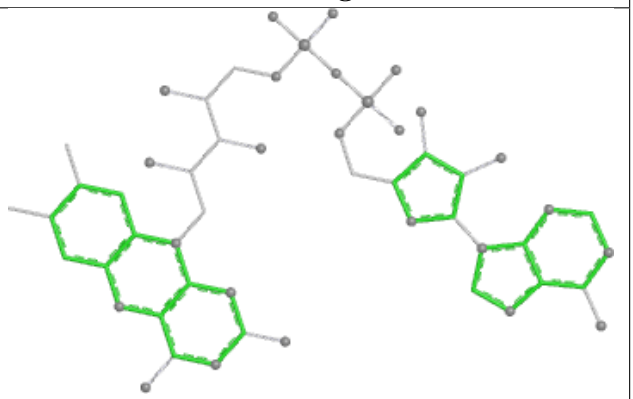
Bond lengths



Bond angles

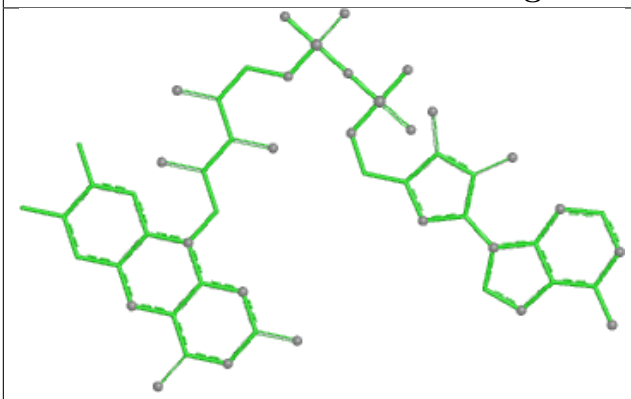


Torsions

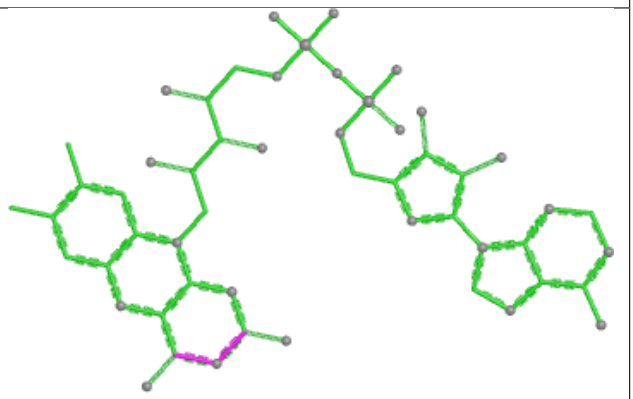


Rings

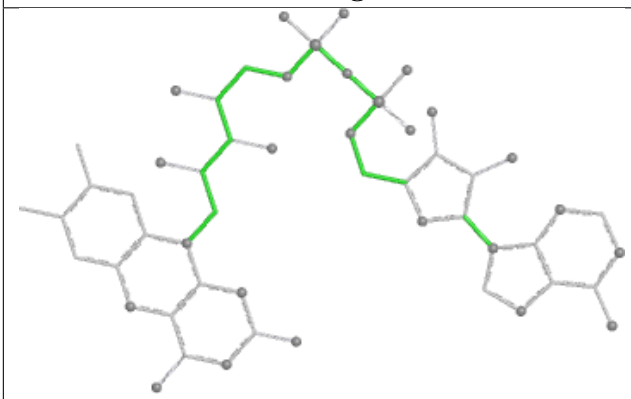
Ligand FAD D 601



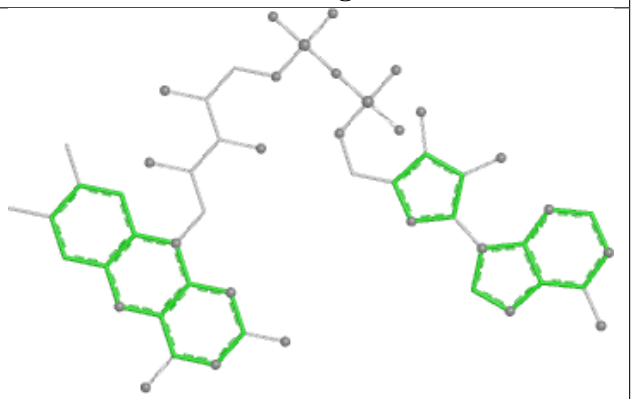
Bond lengths



Bond angles

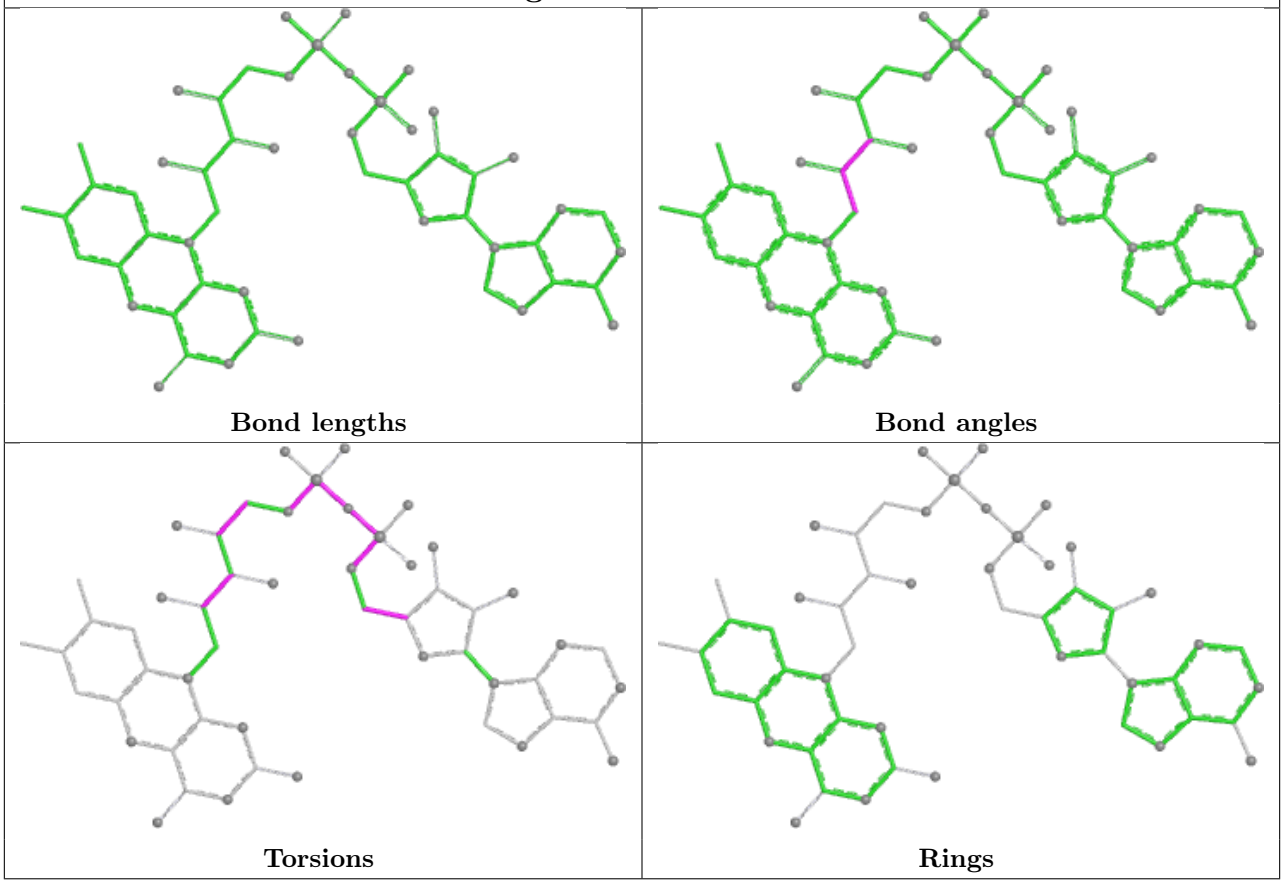


Torsions



Rings

Ligand FAD A 601



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	539/558 (96%)	-0.06	4 (0%)	84	85	15, 25, 42, 63	0
1	B	528/558 (94%)	0.08	9 (1%)	69	73	15, 26, 47, 57	0
1	C	535/558 (95%)	0.18	7 (1%)	75	78	21, 31, 49, 62	0
1	D	527/558 (94%)	0.51	26 (4%)	35	39	22, 35, 54, 74	0
All	All	2129/2232 (95%)	0.18	46 (2%)	62	66	15, 30, 50, 74	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	PHE	3.5
1	B	532	HIS	3.3
1	D	335	LEU	3.3
1	D	457	CYS	2.9
1	B	541	ALA	2.9
1	C	15	PRO	2.8
1	D	203	PRO	2.8
1	B	228	ASP	2.7
1	D	488	ARG	2.7
1	C	189	PHE	2.7
1	D	189	PHE	2.5
1	B	189	PHE	2.5
1	D	438	THR	2.5
1	C	439	GLY	2.5
1	D	519	ASP	2.4
1	D	422	VAL	2.4
1	D	486	ALA	2.4
1	D	202	GLU	2.4
1	D	125	ILE	2.4
1	D	279	ARG	2.4
1	A	523	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	492	GLN	2.3
1	C	549	ALA	2.3
1	D	541	ALA	2.3
1	D	452	TYR	2.3
1	D	442	SER	2.2
1	B	438	THR	2.2
1	D	433	THR	2.2
1	D	489	VAL	2.1
1	D	492	GLN	2.1
1	D	480	HIS	2.1
1	B	530	GLY	2.1
1	D	434	ARG	2.1
1	B	420	ALA	2.1
1	D	336	MET	2.1
1	B	127	GLY	2.1
1	A	165	ASP	2.1
1	D	165	ASP	2.1
1	C	190	ARG	2.1
1	D	482	THR	2.1
1	C	175	GLY	2.1
1	D	425	GLY	2.1
1	D	530	GLY	2.1
1	B	440	ASP	2.0
1	A	188	GLY	2.0
1	D	428	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

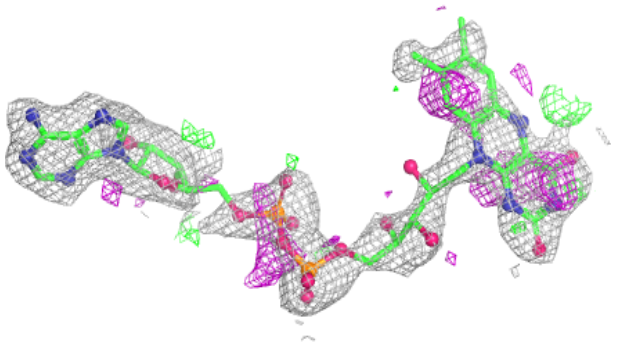
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

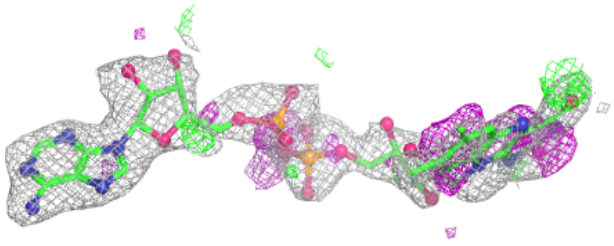
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	C	601	53/53	0.77	0.17	48,57,72,73	0
2	FAD	B	601	53/53	0.80	0.14	39,47,53,55	0
2	FAD	A	601	53/53	0.80	0.16	42,51,60,61	0
2	FAD	D	601	53/53	0.81	0.14	45,56,65,71	0
4	CL	B	604	1/1	0.83	0.42	65,65,65,65	0
6	NA	C	604	1/1	0.87	0.18	51,51,51,51	0
3	GOL	B	602	6/6	0.88	0.13	38,41,42,45	0
5	EPE	C	603	13/15	0.90	0.12	43,45,47,50	0
5	EPE	B	603	15/15	0.91	0.11	37,39,43,45	0
3	GOL	C	602	6/6	0.92	0.09	31,34,34,34	0
4	CL	D	602	1/1	0.93	0.25	59,59,59,59	0
4	CL	C	605	1/1	0.94	0.26	60,60,60,60	0
3	GOL	A	602	6/6	0.95	0.07	24,25,26,26	0
4	CL	A	603	1/1	0.95	0.21	49,49,49,49	0

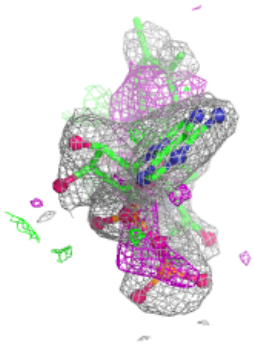
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 601:

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

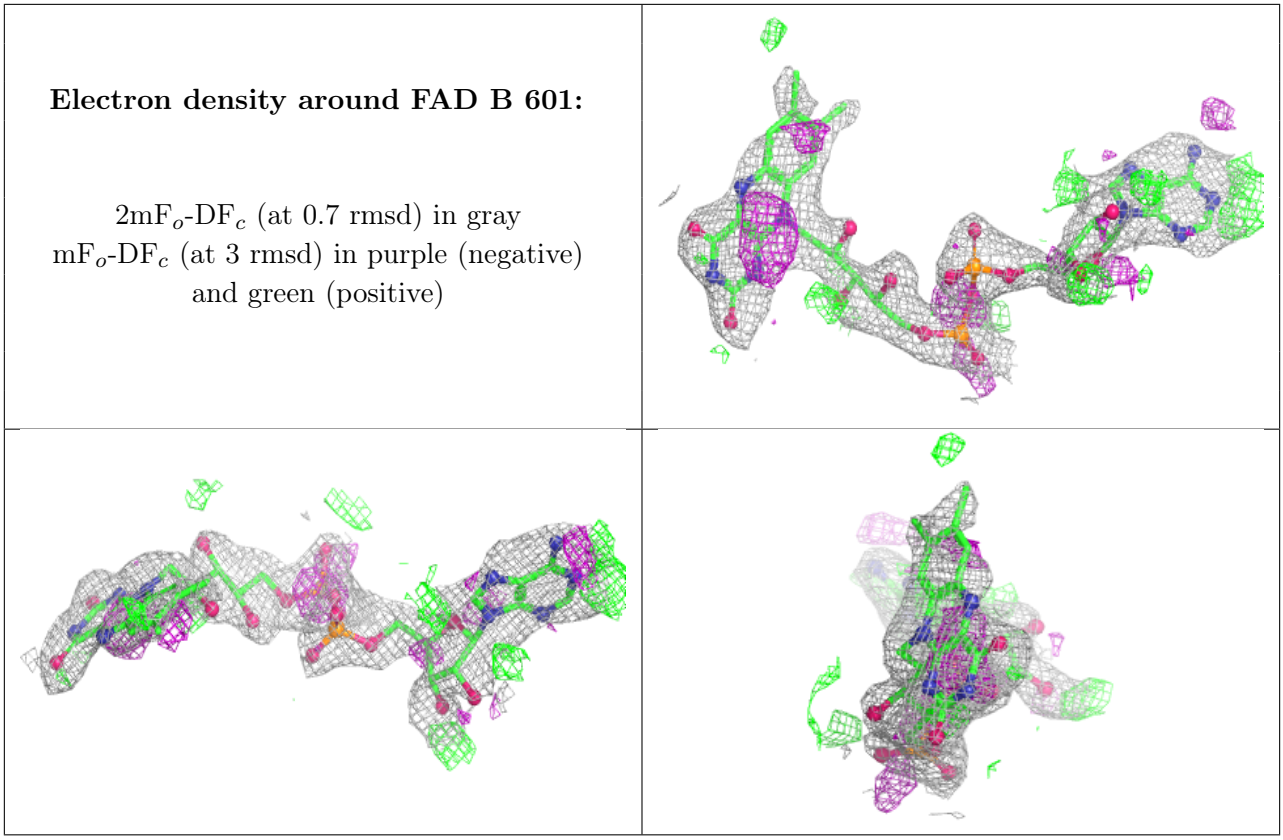






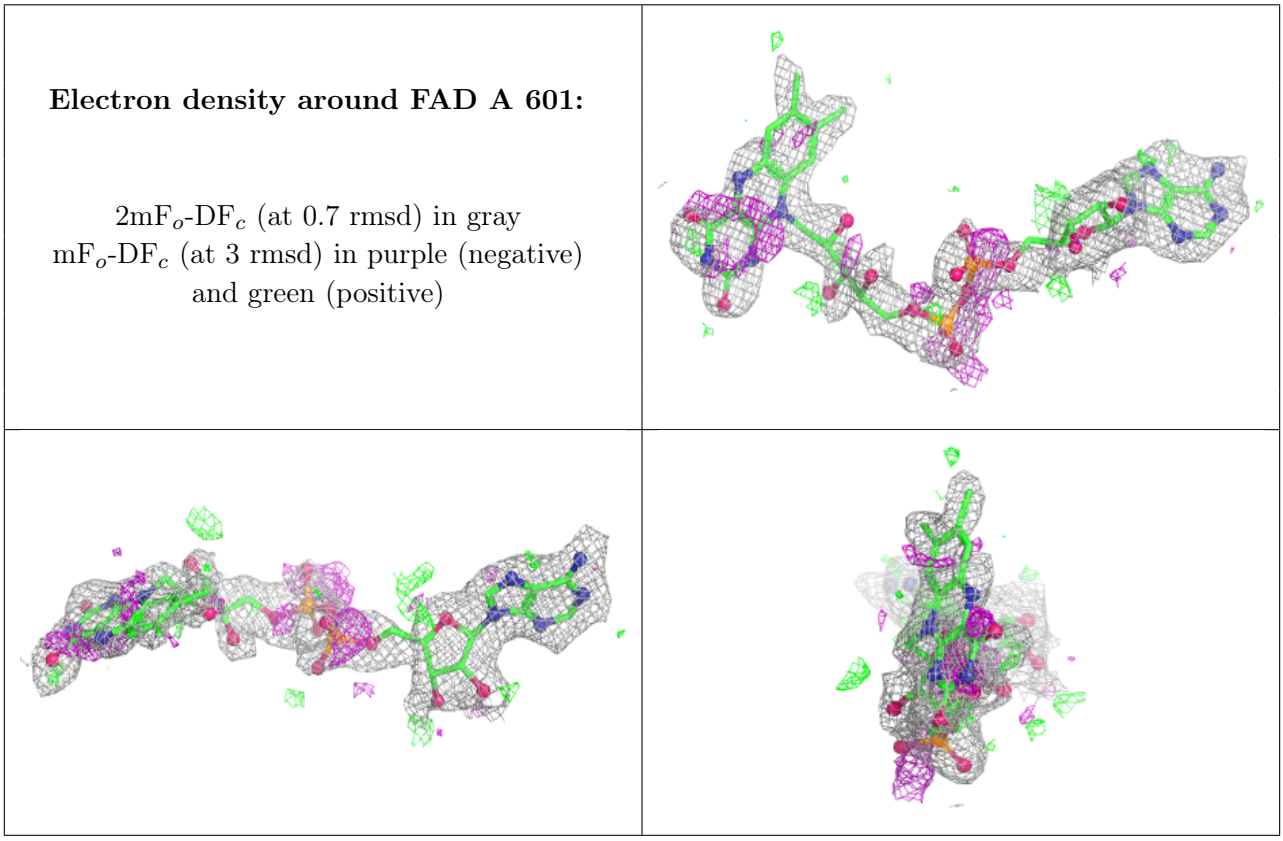
Electron density around FAD B 601:

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



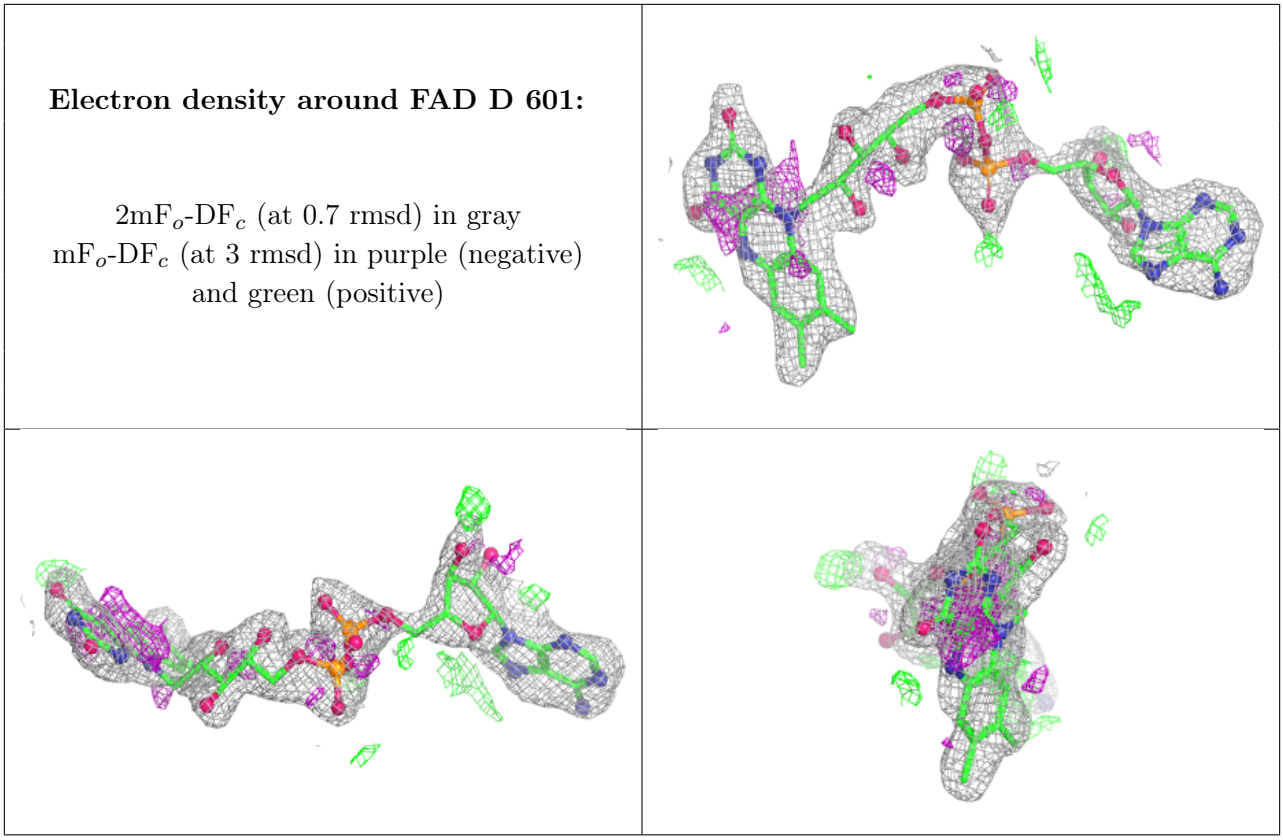
Electron density around FAD A 601:

$2mF_o$-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 601:

$2mF_o$-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.