



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:58 PM BST

PDB ID : 5ZU2
Title : Effect of mutation (R554A) on FAD modification in *Aspergillus oryzae* RIB40formate oxidase
Authors : Mikami, B.; Uchida, H.; Doubayashi, D.
Deposited on : 2018-05-06
Resolution : 2.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

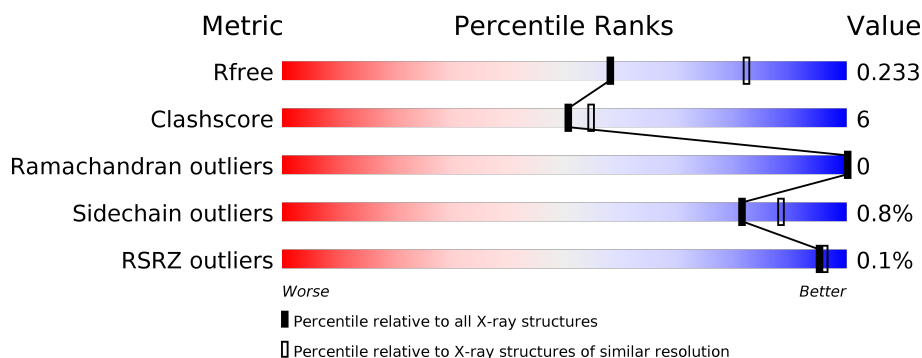
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	577	
1	B	577	
1	C	577	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MPD	A	604	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14187 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.

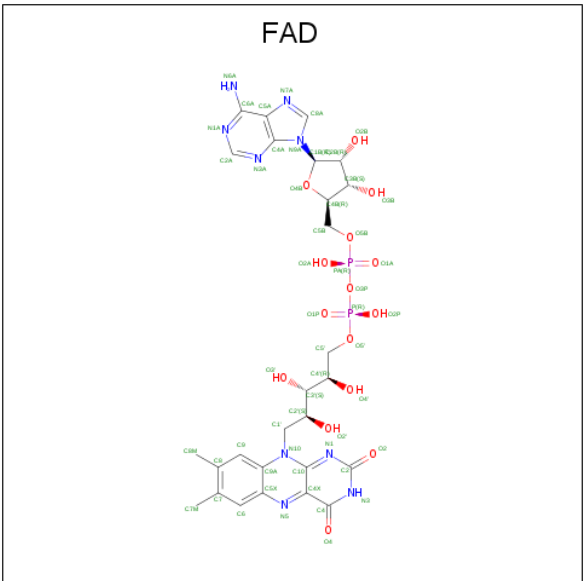
- Molecule 1 is a protein called formate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4521	2867	782	852	20			
1	B	577	Total	C	N	O	S	0	0	0
			4521	2867	782	852	20			
1	C	577	Total	C	N	O	S	1	1	0
			4526	2870	782	854	20			

There are 3 discrepancies between the modelled and reference sequences:

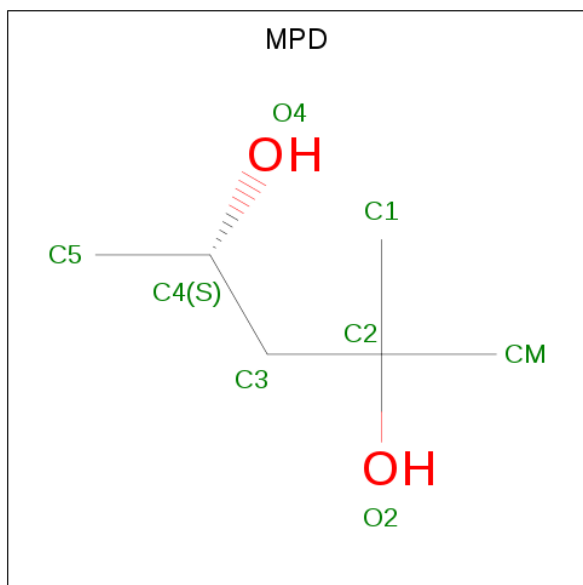
Chain	Residue	Modelled	Actual	Comment	Reference
A	554	ALA	ARG	engineered mutation	UNP Q2UD26
B	554	ALA	ARG	engineered mutation	UNP Q2UD26
C	554	ALA	ARG	engineered mutation	UNP Q2UD26

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by author).



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		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

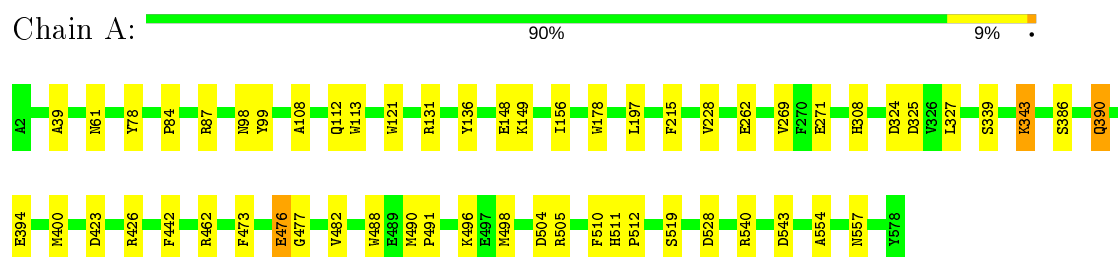
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	191	Total	O	0	0
			191	191		
5	B	132	Total	O	0	0
			132	132		
5	C	93	Total	O	0	0
			93	93		

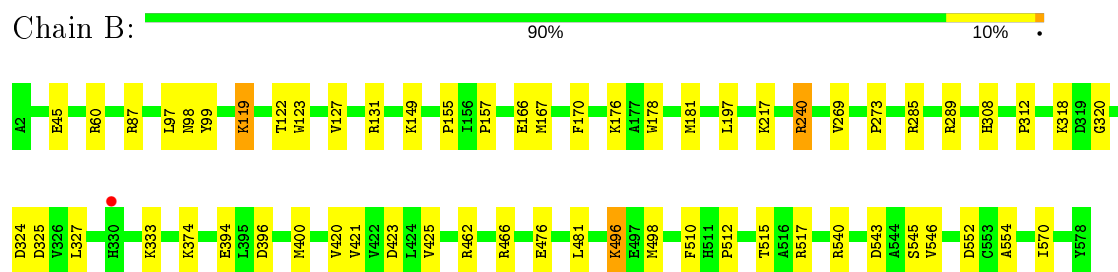
3 Residue-property plots

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.

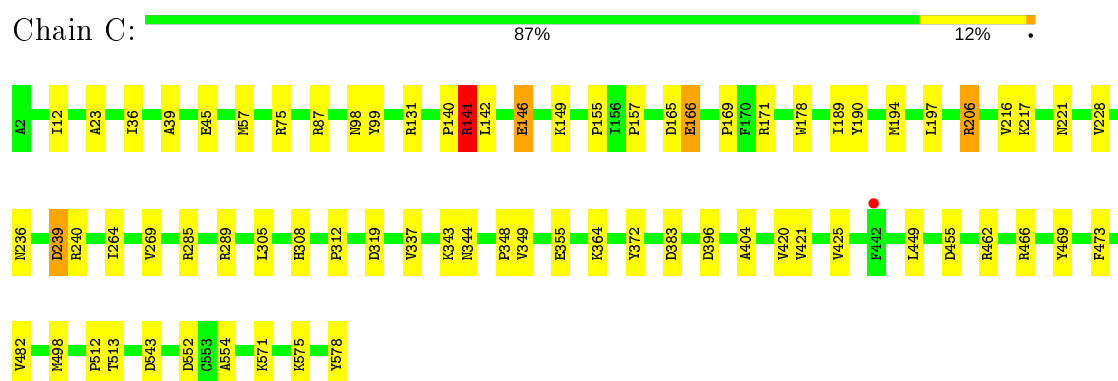
- Molecule 1: formate oxidase



- Molecule 1: formate oxidase



- Molecule 1: formate oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	155.32Å 156.94Å 184.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.83 – 2.44 49.17 – 2.44	Depositor EDS
% Data completeness (in resolution range)	96.5 (38.83-2.44) 96.4 (49.17-2.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.20 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.184 , 0.233 0.184 , 0.233	Depositor DCC
R_{free} test set	3928 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14187	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, FAD, ACT

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	0.45	0/4634	0.64	1/6286 (0.0%)
1	B	0.42	0/4634	0.69	5/6286 (0.1%)
1	C	0.48	4/4642 (0.1%)	0.79	23/6297 (0.4%)
All	All	0.45	4/13910 (0.0%)	0.71	29/18869 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	575	LYS	CD-CE	6.51	1.67	1.51
1	C	146	GLU	CB-CG	6.20	1.64	1.52
1	C	206	ARG	NE-CZ	5.70	1.40	1.33
1	C	146	GLU	CG-CD	5.19	1.59	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	LYS	CD-CE-NZ	-14.44	78.49	111.70
1	B	240	ARG	NE-CZ-NH2	-11.83	114.38	120.30
1	C	166	GLU	CG-CD-OE1	10.76	139.81	118.30
1	C	166	GLU	N-CA-CB	10.17	128.90	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	LYS	CB-CG-CD	-9.53	86.83	111.60
1	C	166	GLU	CG-CD-OE2	-8.81	100.68	118.30
1	C	146	GLU	CB-CA-C	8.23	126.86	110.40
1	C	217	LYS	CA-CB-CG	-7.72	96.42	113.40
1	C	575	LYS	CD-CE-NZ	7.58	129.14	111.70
1	C	166	GLU	CA-CB-CG	7.38	129.64	113.40
1	C	146	GLU	CA-CB-CG	7.20	129.24	113.40
1	C	141	ARG	CB-CG-CD	-7.00	93.40	111.60
1	C	165	ASP	C-N-CA	-6.98	104.25	121.70
1	B	496	LYS	CG-CD-CE	-6.68	91.87	111.90
1	C	206	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	C	141	ARG	CG-CD-NE	6.53	125.52	111.80
1	A	476	GLU	CA-CB-CG	-6.25	99.66	113.40
1	B	240	ARG	CD-NE-CZ	5.94	131.92	123.60
1	C	146	GLU	CB-CG-CD	5.82	129.90	114.20
1	C	45	GLU	CB-CA-C	-5.65	99.11	110.40
1	C	146	GLU	CG-CD-OE1	5.60	129.50	118.30
1	C	45	GLU	CB-CG-CD	5.54	129.16	114.20
1	B	119	LYS	CA-CB-CG	-5.41	101.50	113.40
1	C	206	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	45	GLU	CG-CD-OE2	-5.34	107.61	118.30
1	C	575	LYS	CG-CD-CE	5.29	127.77	111.90
1	C	575	LYS	CB-CG-CD	-5.22	98.03	111.60
1	C	166	GLU	CB-CG-CD	5.19	128.22	114.20
1	C	206	ARG	NH1-CZ-NH2	5.18	125.10	119.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	240	ARG	Sidechain
1	C	513	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4521	0	4435	52	0
1	B	4521	0	4435	46	0
1	C	4526	0	4439	54	0
2	A	53	0	31	10	0
2	B	53	0	31	11	0
2	C	53	0	31	6	0
3	A	24	0	42	12	0
3	B	8	0	14	0	0
3	C	8	0	14	1	0
4	A	4	0	3	1	0
5	A	191	0	0	2	0
5	B	132	0	0	5	0
5	C	93	0	0	4	0
All	All	14187	0	13475	156	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 6.

All (156) 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:A:308:HIS:HD2	1:A:511:HIS:HD2	1.16	0.92
1:C:75:ARG:NH2	1:C:455:ASP:OD1	2.02	0.91
1:B:325:ASP:OD2	1:B:333:LYS:NZ	2.04	0.89
1:A:476:GLU:HG3	1:A:477:GLY:N	1.87	0.88
1:B:119:LYS:O	1:B:119:LYS:HG3	1.73	0.86
1:A:308:HIS:HD2	1:A:511:HIS:CD2	1.98	0.80
1:A:308:HIS:CD2	1:A:511:HIS:HD2	2.03	0.76
1:C:57:MET:HE2	1:C:404:ALA:H	1.51	0.75
1:B:166:GLU:OE1	5:B:701:HOH:O	2.05	0.74
1:A:505:ARG:NE	3:A:604:MPD:H52	2.05	0.71
1:C:141:ARG:HD2	1:C:141:ARG:N	2.05	0.70
1:C:337:VAL:HG13	1:C:348:PRO:HD2	1.72	0.69
1:A:386:SER:HB3	1:A:390:GLN:HG2	1.75	0.68
1:C:240:ARG:NH1	5:C:701:HOH:O	2.27	0.67
1:B:554:ALA:HB1	2:B:601:FAD:C2	2.25	0.67
1:B:320:GLY:O	5:B:701:HOH:O	2.13	0.67
1:A:505:ARG:HE	3:A:604:MPD:H52	1.61	0.65
1:C:236:ASN:ND2	1:C:239:ASP:HB2	2.13	0.64
1:A:156:ILE:HD11	1:A:215:PHE:HE2	1.63	0.64
1:C:554:ALA:HB1	2:C:601:FAD:C2	2.26	0.64
1:C:57:MET:HE3	1:C:404:ALA:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LEU:HB2	1:B:400:MET:CE	2.29	0.61
1:A:324:ASP:HA	1:A:400:MET:HE2	1.81	0.61
1:A:339:SER:O	1:A:343:LYS:HE2	2.01	0.61
1:A:505:ARG:HH21	3:A:604:MPD:C5	2.12	0.61
1:C:206:ARG:HD2	5:C:786:HOH:O	2.02	0.60
1:C:469:TYR:HB3	3:C:602:MPD:H51	1.84	0.60
1:C:12:ILE:HG13	1:C:23:ALA:HB2	1.84	0.60
1:B:394:GLU:O	1:B:423:ASP:HB3	2.03	0.59
1:A:98:ASN:HB2	2:A:601:FAD:C5X	2.31	0.59
1:C:554:ALA:HB1	2:C:601:FAD:N3	2.18	0.59
1:C:189:ILE:HG22	1:C:194:MET:HA	1.85	0.58
1:C:240:ARG:HG3	1:C:240:ARG:HH11	1.69	0.58
1:C:337:VAL:HG12	1:C:349:VAL:HG23	1.85	0.57
1:C:473:PHE:CE2	1:C:482:VAL:HG11	2.39	0.57
1:B:178:TRP:CE2	1:B:197:LEU:HB2	2.40	0.57
1:A:156:ILE:HD11	1:A:215:PHE:CE2	2.40	0.56
1:B:396:ASP:HB2	1:B:421:VAL:HB	1.87	0.56
1:C:396:ASP:HB2	1:C:421:VAL:HB	1.86	0.56
1:A:505:ARG:NH2	3:A:604:MPD:C5	2.68	0.56
1:B:327:LEU:HB2	1:B:400:MET:HE1	1.87	0.56
1:C:343:LYS:HD2	1:C:344:ASN:HB3	1.86	0.56
1:B:167:MET:HE3	1:B:170:PHE:CB	2.36	0.55
1:C:98:ASN:HB2	2:C:601:FAD:C5X	2.37	0.55
1:A:554:ALA:HB1	2:A:601:FAD:C2	2.37	0.55
1:C:305:LEU:HD21	1:C:449:LEU:HD23	1.89	0.55
1:C:206:ARG:HG2	1:C:206:ARG:NH2	2.21	0.54
1:B:123:TRP:O	1:B:127:VAL:HG23	2.08	0.53
1:B:318:LYS:HG3	1:B:481:LEU:O	2.09	0.53
1:B:99:TYR:CD2	2:B:601:FAD:H6	2.44	0.53
1:A:505:ARG:NH2	3:A:604:MPD:H51	2.24	0.53
1:C:155:PRO:O	1:C:157:PRO:HD3	2.09	0.52
1:C:12:ILE:HD13	1:C:264:ILE:HB	1.91	0.52
1:A:262:GLU:OE1	1:A:540:ARG:HD2	2.09	0.52
1:B:98:ASN:HB2	2:B:601:FAD:C5X	2.40	0.51
1:B:308:HIS:CD2	1:B:425:VAL:HA	2.46	0.50
1:B:119:LYS:HE2	1:B:122:THR:OG1	2.11	0.50
1:C:206:ARG:HG2	1:C:206:ARG:HH21	1.77	0.50
1:B:45:GLU:H	1:B:45:GLU:CD	2.16	0.50
1:A:61:ASN:OD1	1:A:84:PRO:HG3	2.12	0.49
1:A:269:VAL:HG11	1:A:512:PRO:HB2	1.93	0.49
1:C:285:ARG:O	1:C:289:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:VAL:HG11	1:C:512:PRO:HG2	1.95	0.49
1:B:510:PHE:HB3	2:B:601:FAD:C9	2.43	0.49
1:A:543:ASP:HB2	2:A:601:FAD:O2P	2.13	0.49
1:B:318:LYS:HD3	1:B:481:LEU:HA	1.93	0.49
1:A:488:TRP:HE1	3:A:604:MPD:H4	1.79	0.48
1:A:442:PHE:O	4:A:605:ACT:H2	2.14	0.48
1:C:240:ARG:CG	1:C:240:ARG:HH11	2.27	0.48
1:A:327:LEU:HB2	1:A:400:MET:CE	2.43	0.48
1:B:98:ASN:HA	2:B:601:FAD:C6	2.44	0.48
1:B:119:LYS:O	1:B:119:LYS:CG	2.52	0.48
1:C:337:VAL:CG1	1:C:349:VAL:HG23	2.44	0.48
1:B:462:ARG:HD3	1:B:466:ARG:NH2	2.29	0.47
1:C:166:GLU:O	1:C:169:PRO:HD2	2.14	0.47
1:A:554:ALA:HB1	2:A:601:FAD:N3	2.29	0.47
1:C:473:PHE:CZ	1:C:482:VAL:HG11	2.50	0.47
1:A:178:TRP:CE2	1:A:197:LEU:HB2	2.50	0.47
1:A:394:GLU:O	1:A:423:ASP:HB3	2.14	0.47
1:B:176:LYS:HG2	1:B:476:GLU:OE2	2.14	0.47
1:B:327:LEU:HB2	1:B:400:MET:HE3	1.96	0.47
1:B:510:PHE:HB3	2:B:601:FAD:C8	2.45	0.47
1:B:269:VAL:HA	1:B:545:SER:HB3	1.96	0.46
3:A:604:MPD:H32	5:A:872:HOH:O	2.15	0.46
1:B:155:PRO:O	1:B:157:PRO:HD3	2.15	0.46
1:B:98:ASN:HB2	2:B:601:FAD:N5	2.30	0.46
1:B:374:LYS:NZ	5:B:712:HOH:O	2.46	0.46
1:B:269:VAL:HG11	1:B:512:PRO:HB2	1.97	0.46
1:C:372:TYR:OH	1:C:383:ASP:OD1	2.25	0.46
1:C:87:ARG:NH1	5:C:705:HOH:O	2.48	0.46
1:A:505:ARG:HH21	3:A:604:MPD:H51	1.80	0.46
1:C:337:VAL:HG11	1:C:348:PRO:HG2	1.98	0.45
1:A:476:GLU:HG3	1:A:477:GLY:H	1.76	0.45
1:C:171:ARG:NH1	1:C:355:GLU:OE1	2.47	0.45
1:A:131:ARG:HD3	1:A:149:LYS:O	2.17	0.45
1:A:113:TRP:HB2	1:A:121:TRP:O	2.16	0.45
1:C:140:PRO:HB2	1:C:142:LEU:HG	1.98	0.45
1:A:505:ARG:CZ	3:A:604:MPD:H52	2.47	0.45
1:A:473:PHE:CZ	1:A:482:VAL:HG11	2.51	0.45
3:A:602:MPD:H13	5:A:711:HOH:O	2.17	0.45
1:B:87:ARG:NH2	2:B:601:FAD:HM81	2.31	0.45
1:A:308:HIS:CD2	1:A:511:HIS:CD2	2.87	0.45
1:C:364:LYS:HE2	5:C:715:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ALA:HA	1:A:228:VAL:O	2.18	0.44
1:A:390:GLN:HG3	1:A:426:ARG:HD2	1.99	0.44
1:A:98:ASN:HB2	2:A:601:FAD:N5	2.33	0.44
1:B:167:MET:HE3	1:B:170:PHE:CG	2.53	0.44
1:C:543:ASP:HB2	2:C:601:FAD:O2P	2.17	0.43
1:A:87:ARG:NH2	2:A:601:FAD:HM81	2.33	0.43
1:C:308:HIS:CD2	1:C:425:VAL:HA	2.53	0.43
1:A:327:LEU:HB2	1:A:400:MET:HE1	2.01	0.43
1:B:285:ARG:O	1:B:289:ARG:HG3	2.19	0.43
1:B:181:MET:HE2	5:B:818:HOH:O	2.18	0.43
1:B:273:PRO:HG3	1:B:515:THR:HB	2.00	0.43
1:C:462:ARG:HD3	1:C:466:ARG:NH2	2.32	0.43
1:A:269:VAL:HG11	1:A:512:PRO:HG2	2.01	0.43
2:B:601:FAD:H1'1	2:B:601:FAD:H9	1.82	0.43
1:C:39:ALA:HA	1:C:228:VAL:O	2.19	0.42
1:C:462:ARG:HG3	1:C:498:MET:HB3	2.02	0.42
1:C:571:LYS:HG2	1:C:578:TYR:CD2	2.55	0.42
1:C:98:ASN:HB2	2:C:601:FAD:N5	2.34	0.42
1:B:324:ASP:HA	1:B:400:MET:HE2	2.02	0.42
1:C:131:ARG:HH12	1:C:149:LYS:HD2	1.84	0.42
1:A:519:SER:O	1:A:528:ASP:HA	2.20	0.42
1:A:98:ASN:HA	2:A:601:FAD:C6	2.50	0.42
1:B:131:ARG:HH12	1:B:149:LYS:HD2	1.84	0.42
1:B:98:ASN:HB2	2:B:601:FAD:C4X	2.49	0.42
1:A:78:TYR:OH	1:A:504:ASP:HA	2.19	0.41
1:B:517:ARG:HA	1:B:546:VAL:HA	2.01	0.41
1:C:12:ILE:CD1	1:C:264:ILE:HB	2.50	0.41
1:C:240:ARG:CG	1:C:240:ARG:NH1	2.83	0.41
1:A:99:TYR:CD2	2:A:601:FAD:H6	2.55	0.41
1:A:490:MET:HE2	1:A:498:MET:SD	2.61	0.41
1:A:510:PHE:HB3	2:A:601:FAD:C8	2.50	0.41
1:A:490:MET:CE	1:A:491:PRO:HD2	2.50	0.41
1:B:462:ARG:HG3	1:B:498:MET:HB3	2.01	0.41
1:C:312:PRO:HA	1:C:420:VAL:O	2.20	0.41
1:B:540:ARG:NE	1:B:570:ILE:HG12	2.35	0.41
1:C:178:TRP:CE2	1:C:197:LEU:HB2	2.55	0.41
1:C:99:TYR:CD2	2:C:601:FAD:H6	2.56	0.41
1:A:136:TYR:CD2	1:A:148:GLU:HA	2.56	0.41
1:A:488:TRP:HE1	3:A:604:MPD:C4	2.33	0.41
3:A:604:MPD:HM1	3:A:604:MPD:H4	1.88	0.41
1:B:543:ASP:HB2	2:B:601:FAD:O2P	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ASN:OD1	1:C:221:ASN:N	2.47	0.41
1:C:190:TYR:N	1:C:190:TYR:CD1	2.88	0.41
1:A:108:ALA:O	1:A:112:GLN:HG2	2.21	0.40
1:C:57:MET:CE	1:C:404:ALA:HB3	2.49	0.40
1:B:312:PRO:HA	1:B:420:VAL:O	2.21	0.40
1:A:490:MET:HE2	1:A:491:PRO:HD2	2.04	0.40
1:A:462:ARG:HG3	1:A:498:MET:HB3	2.03	0.40
1:A:271:GLU:HG3	2:A:601:FAD:N7A	2.37	0.40
1:B:60:ARG:HD2	5:B:746:HOH:O	2.21	0.40
1:B:167:MET:HE3	1:B:170:PHE:HB3	2.02	0.40
1:C:36:ILE:HD11	1:C:216:VAL:HG11	2.04	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	575/577 (100%)	555 (96%)	20 (4%)	0	100	100
1	B	575/577 (100%)	557 (97%)	18 (3%)	0	100	100
1	C	576/577 (100%)	557 (97%)	19 (3%)	0	100	100
All	All	1726/1731 (100%)	1669 (97%)	57 (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	A	491/491 (100%)	486 (99%)	5 (1%)	76	84
1	B	491/491 (100%)	488 (99%)	3 (1%)	86	91
1	C	492/491 (100%)	488 (99%)	4 (1%)	81	88
All	All	1474/1473 (100%)	1462 (99%)	12 (1%)	81	88

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	ASP
1	A	343	LYS
1	A	390	GLN
1	A	496	LYS
1	A	557	ASN
1	B	97	LEU
1	B	496	LYS
1	B	552	ASP
1	C	141	ARG
1	C	146	GLU
1	C	239	ASP
1	C	552	ASP

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

Mol	Chain	Res	Type
1	A	308	HIS
1	A	511	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	A	605	-	1,3,3	9.33	1 (100%)	0,3,3	0.00	-
2	FAD	C	601	-	51,58,58	1.35	5 (9%)	60,89,89	2.24	7 (11%)
2	FAD	A	601	-	51,58,58	1.35	4 (7%)	60,89,89	2.27	7 (11%)
2	FAD	B	601	-	51,58,58	1.30	5 (9%)	60,89,89	2.22	7 (11%)
3	MPD	A	603	-	7,7,7	0.59	0	9,10,10	0.64	0
3	MPD	B	602	-	7,7,7	0.32	0	9,10,10	0.65	0
3	MPD	A	602	-	7,7,7	0.38	0	9,10,10	0.55	0
3	MPD	C	602	-	7,7,7	0.30	0	9,10,10	0.56	0
3	MPD	A	604	-	7,7,7	0.49	0	9,10,10	0.83	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	C	601	-	-	1/30/50/50	0/6/6/6
2	FAD	A	601	-	-	3/30/50/50	0/6/6/6
2	FAD	B	601	-	-	5/30/50/50	0/6/6/6
3	MPD	A	603	-	-	4/5/5/5	-
3	MPD	B	602	-	-	5/5/5/5	-
3	MPD	A	602	-	-	2/5/5/5	-
3	MPD	C	602	-	-	1/5/5/5	-
3	MPD	A	604	-	-	2/5/5/5	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	ACT	CH3-C	9.33	1.60	1.48
2	C	601	FAD	C4X-C10	6.21	1.45	1.38
2	A	601	FAD	C4X-C10	6.12	1.44	1.38
2	B	601	FAD	C4X-C10	5.91	1.44	1.38
2	A	601	FAD	C4-N3	3.94	1.39	1.33
2	C	601	FAD	C4-N3	3.70	1.39	1.33
2	B	601	FAD	C4-N3	3.30	1.38	1.33
2	B	601	FAD	C4-C4X	2.97	1.46	1.41
2	A	601	FAD	C4-C4X	2.93	1.46	1.41
2	B	601	FAD	C5X-N5	2.93	1.40	1.35
2	C	601	FAD	C4-C4X	2.90	1.46	1.41
2	C	601	FAD	C5X-N5	2.69	1.39	1.35
2	A	601	FAD	C9A-N10	2.65	1.42	1.38
2	B	601	FAD	C9A-N10	2.58	1.42	1.38
2	C	601	FAD	C9A-N10	2.48	1.41	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C4-N3-C2	13.05	126.16	115.14
2	B	601	FAD	C4-N3-C2	13.01	126.13	115.14
2	A	601	FAD	C4-N3-C2	12.99	126.11	115.14
2	A	601	FAD	C4X-C4-N3	-7.39	113.32	123.43
2	C	601	FAD	C4X-C4-N3	-7.25	113.52	123.43
2	B	601	FAD	C4X-C4-N3	-6.97	113.90	123.43
2	A	601	FAD	C10-C4X-N5	4.42	124.32	121.26
2	C	601	FAD	C10-C4X-N5	4.32	124.25	121.26
2	B	601	FAD	C10-C4X-N5	4.20	124.16	121.26
2	B	601	FAD	C4-C4X-C10	-3.84	117.41	119.95
2	A	601	FAD	C1'-N10-C9A	3.64	121.16	118.29
2	C	601	FAD	C4-C4X-C10	-3.61	117.56	119.95
2	A	601	FAD	C4X-C10-N10	-3.50	116.70	120.30
2	A	601	FAD	C4-C4X-C10	-3.49	117.64	119.95
2	C	601	FAD	C4X-C10-N10	-3.37	116.84	120.30
2	B	601	FAD	C4X-C10-N10	-3.35	116.86	120.30
2	C	601	FAD	C1'-N10-C9A	3.07	120.71	118.29
2	B	601	FAD	C1'-N10-C9A	2.62	120.36	118.29
2	B	601	FAD	C5A-C6A-N6A	2.34	123.91	120.35
2	C	601	FAD	C5A-C6A-N6A	2.24	123.76	120.35
2	A	601	FAD	C5A-C6A-N6A	2.01	123.41	120.35

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C2'-C1'-N10-C9A
2	B	601	FAD	PA-O3P-P-O5'
3	B	602	MPD	C1-C2-C3-C4
3	B	602	MPD	O2-C2-C3-C4
3	B	602	MPD	C2-C3-C4-O4
3	A	602	MPD	C2-C3-C4-O4
2	B	601	FAD	P-O3P-PA-O1A
3	B	602	MPD	C2-C3-C4-C5
3	A	602	MPD	C2-C3-C4-C5
3	C	602	MPD	C2-C3-C4-C5
3	A	603	MPD	CM-C2-C3-C4
3	B	602	MPD	CM-C2-C3-C4
3	A	604	MPD	C1-C2-C3-C4
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	P-O3P-PA-O1A
2	A	601	FAD	PA-O3P-P-O5'
3	A	603	MPD	O2-C2-C3-C4
2	B	601	FAD	P-O3P-PA-O2A
3	A	603	MPD	C2-C3-C4-C5
3	A	604	MPD	C2-C3-C4-C5
3	A	603	MPD	C2-C3-C4-O4

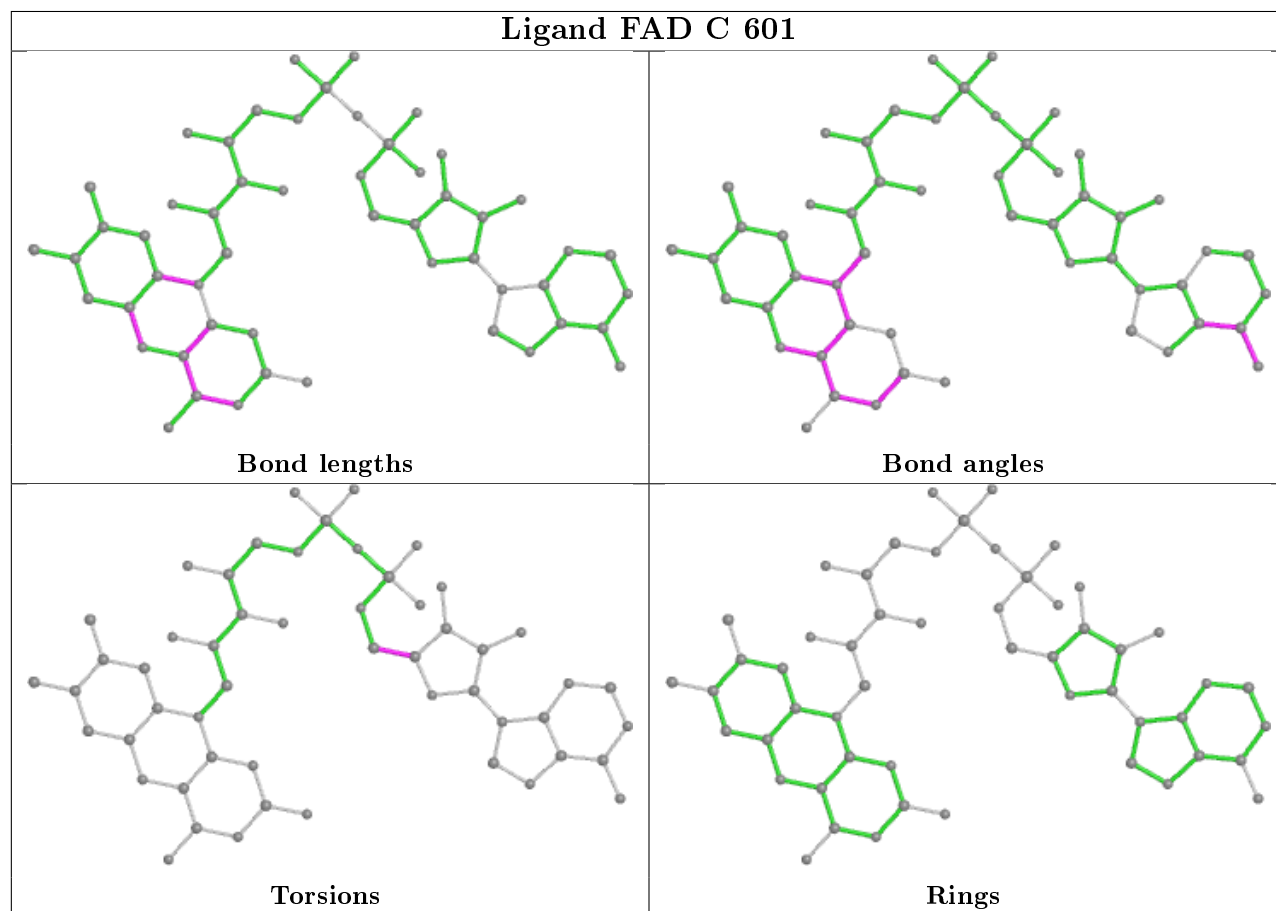
There are no ring outliers.

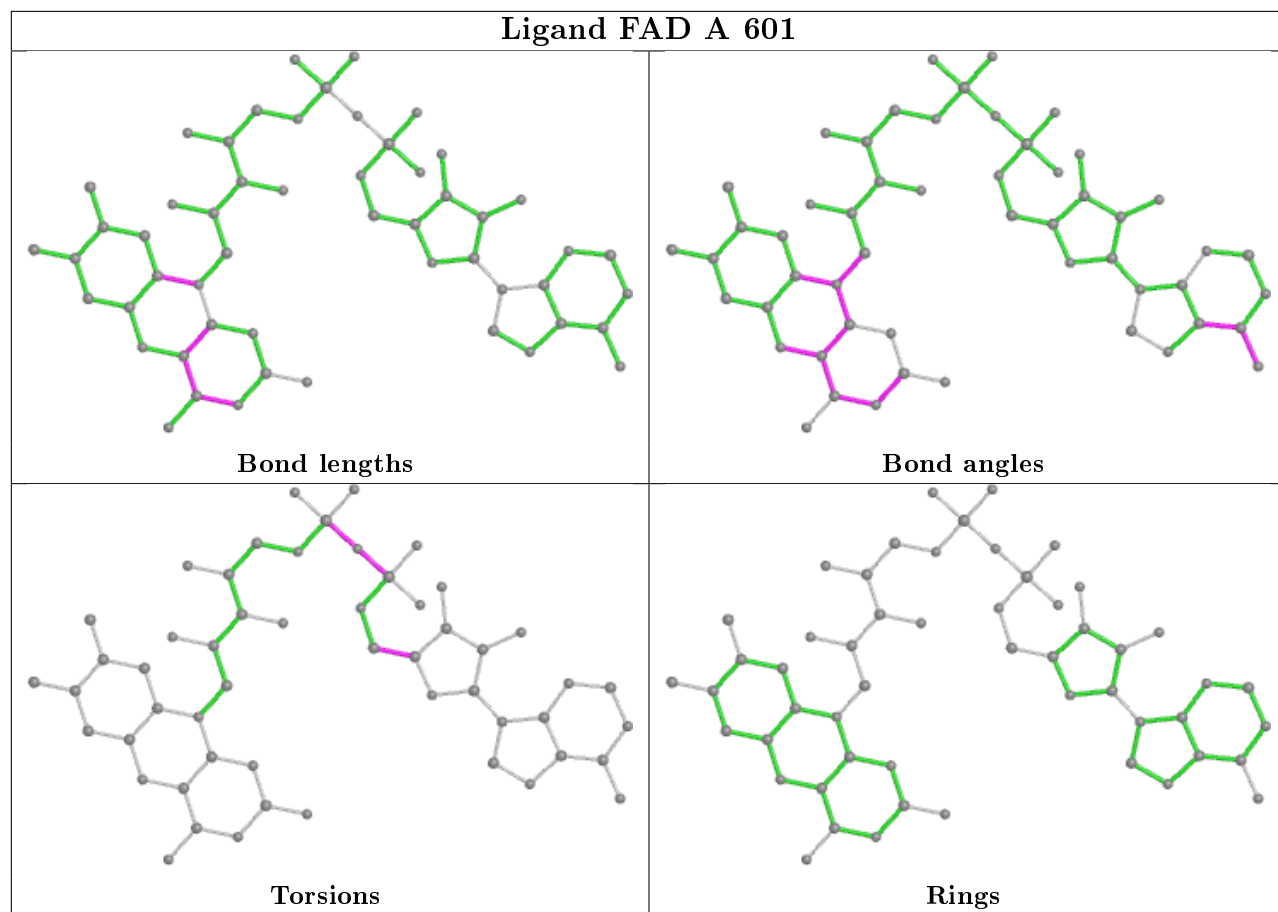
7 monomers are involved in 41 short contacts:

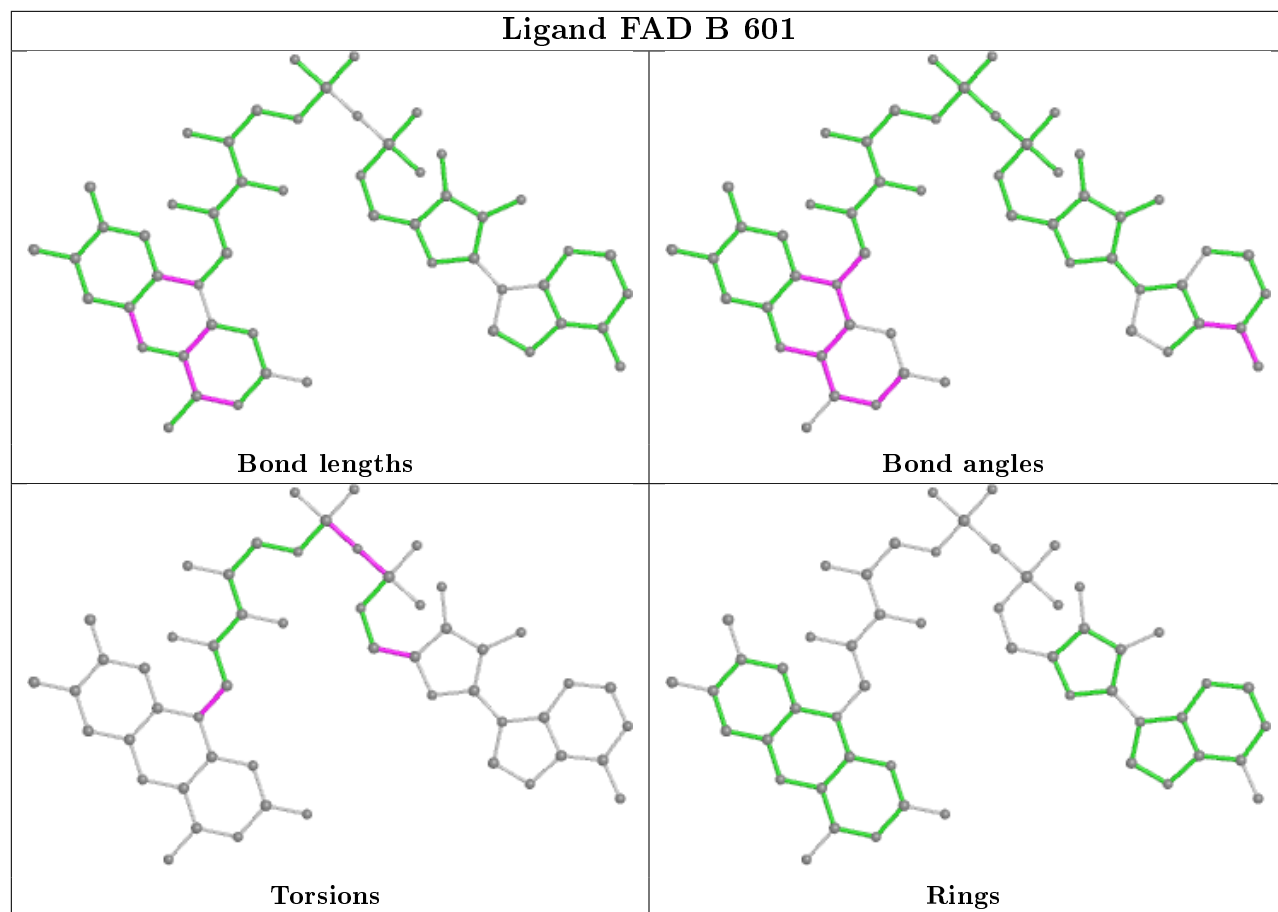
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	ACT	1	0
2	C	601	FAD	6	0
2	A	601	FAD	10	0
2	B	601	FAD	11	0
3	A	602	MPD	1	0
3	C	602	MPD	1	0
3	A	604	MPD	11	0

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.







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	577/577 (100%)	-0.75	0 100 100	20, 27, 40, 54	1 (0%)
1	B	577/577 (100%)	-0.53	1 (0%) 95 95	22, 34, 53, 73	0
1	C	577/577 (100%)	-0.46	1 (0%) 95 95	24, 41, 58, 77	1 (0%)
All	All	1731/1731 (100%)	-0.58	2 (0%) 95 96	20, 33, 54, 77	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	442	PHE	2.3
1	B	330	HIS	2.1

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 monosaccharides 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.

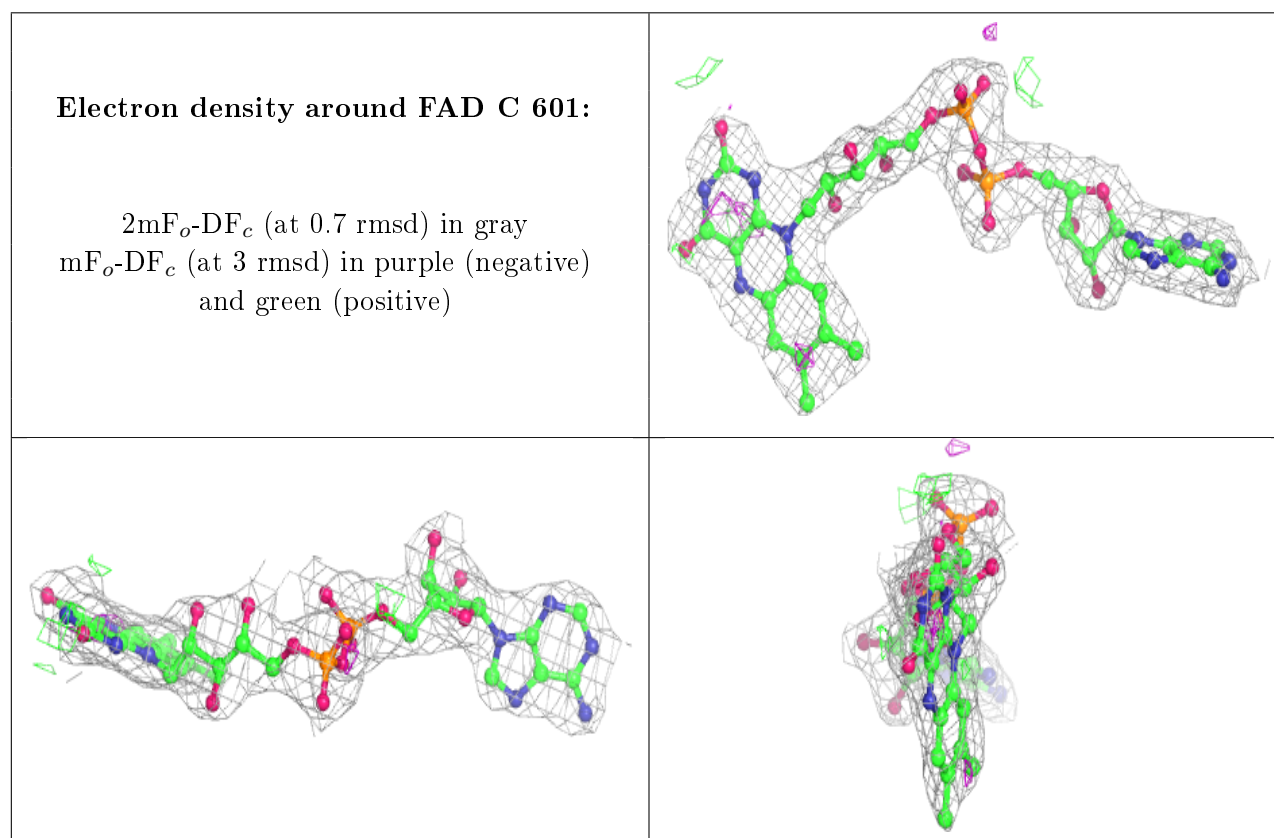
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MPD	A	603	8/8	0.77	0.24	31,39,50,51	0

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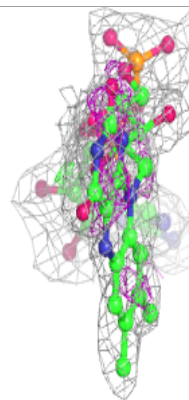
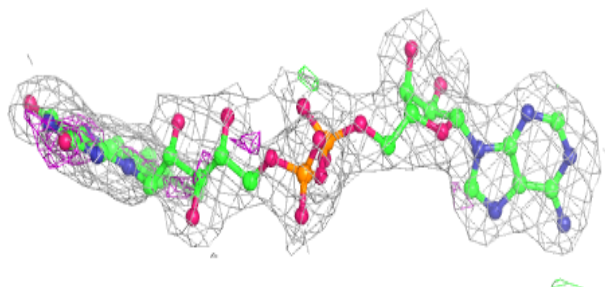
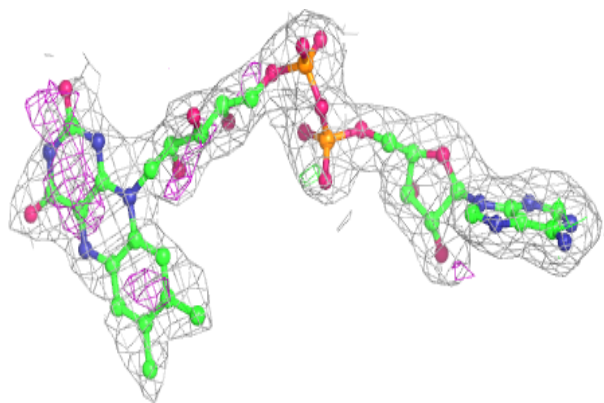
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MPD	A	604	8/8	0.78	0.30	25,37,42,45	0
3	MPD	B	602	8/8	0.82	0.30	41,54,57,59	0
3	MPD	A	602	8/8	0.93	0.13	36,40,48,48	0
4	ACT	A	605	4/4	0.95	0.31	36,37,38,39	0
2	FAD	C	601	53/53	0.96	0.12	26,40,48,51	0
3	MPD	C	602	8/8	0.96	0.18	33,39,43,44	0
2	FAD	A	601	53/53	0.96	0.13	20,25,35,36	0
2	FAD	B	601	53/53	0.97	0.13	20,28,42,46	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.

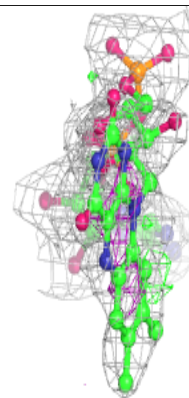
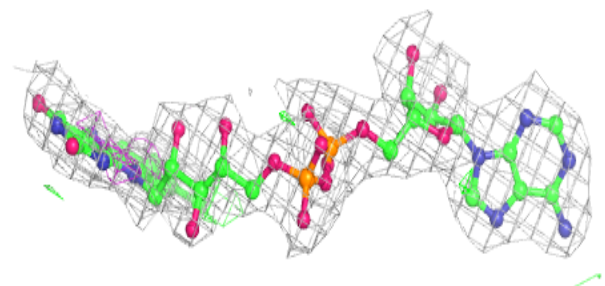
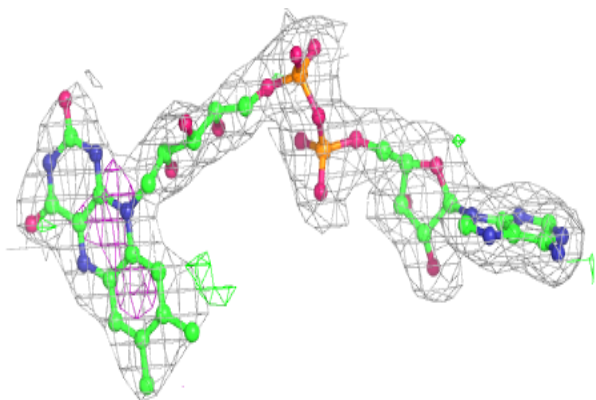


Electron density around FAD A 601:

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

**Electron density around FAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.