



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:04 PM UTC

PDB ID : 6F32 / pdb_00006f32
Title : Crystal structure of a dual function amine oxidase/cyclase in complex with substrate analogues
Authors : Dorival, J.; Risser, F.; Jacob, C.; Collin, S.; Drager, G.; Kirschning, A.; Paris, C.; Chagot, B.; Gruez, A.; Weissman, K.J.
Deposited on : 2017-11-27
Resolution : 2.80 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

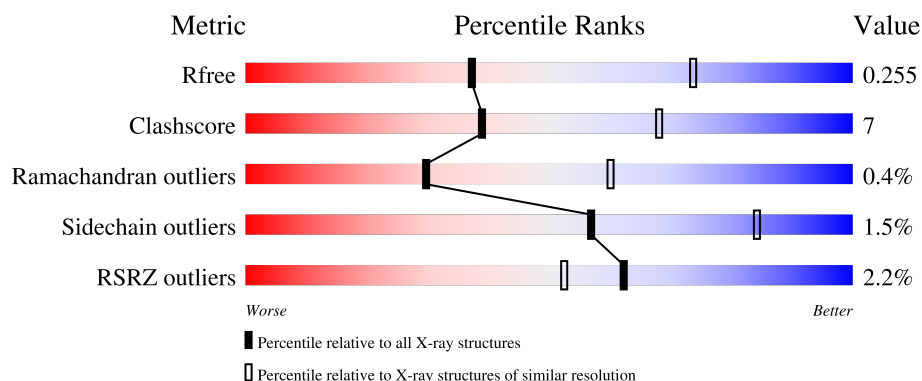
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

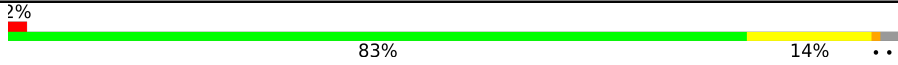
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	A	442	
1	B	442	

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
6	GOL	B	611	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7225 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.

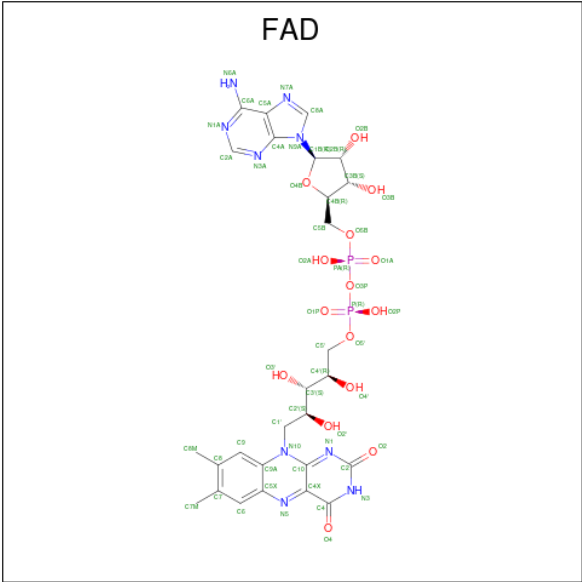
- Molecule 1 is a protein called Amine oxidase LkcE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3431	2175	600	641	15			
1	B	431	Total	C	N	O	S	0	1	0
			3418	2168	599	637	14			

There are 12 discrepancies between the modelled and reference sequences:

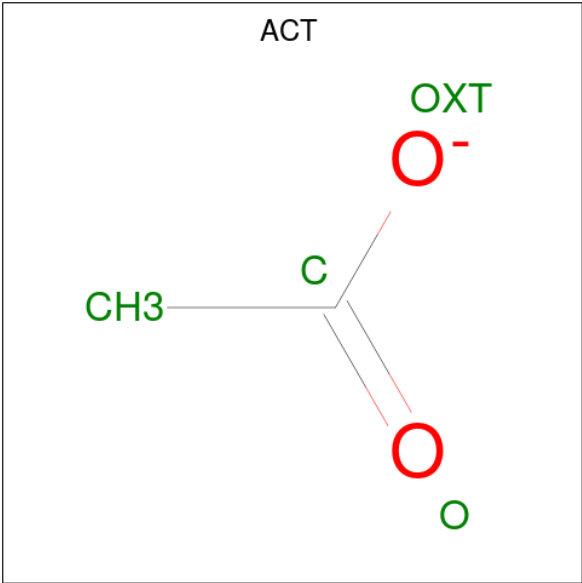
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q83X90
A	-2	PRO	-	expression tag	UNP Q83X90
A	-1	GLY	-	expression tag	UNP Q83X90
A	0	SER	-	expression tag	UNP Q83X90
A	54	GLN	ARG	conflict	UNP Q83X90
A	424	PRO	LEU	conflict	UNP Q83X90
B	-3	GLY	-	expression tag	UNP Q83X90
B	-2	PRO	-	expression tag	UNP Q83X90
B	-1	GLY	-	expression tag	UNP Q83X90
B	0	SER	-	expression tag	UNP Q83X90
B	54	GLN	ARG	conflict	UNP Q83X90
B	424	PRO	LEU	conflict	UNP Q83X90

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



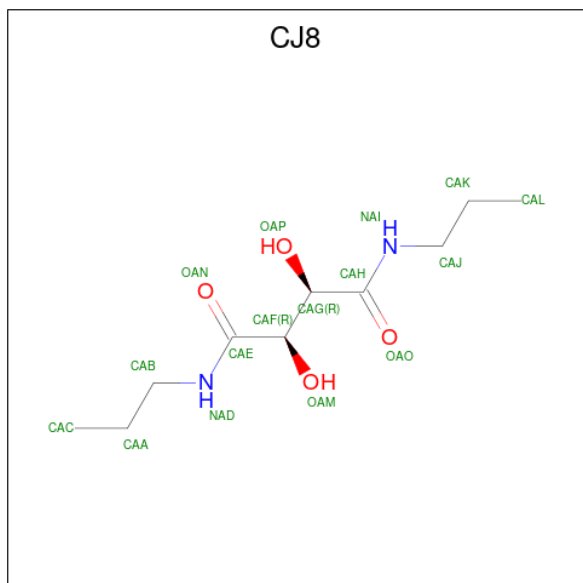
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 4 is (2 {R},3 {R})-2,3-bis(oxidanyl)- {N}, {N}'-dipropyl-butanediamide (CCD ID: CJ8) (formula: C₁₀H₂₀N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	10	2	4		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

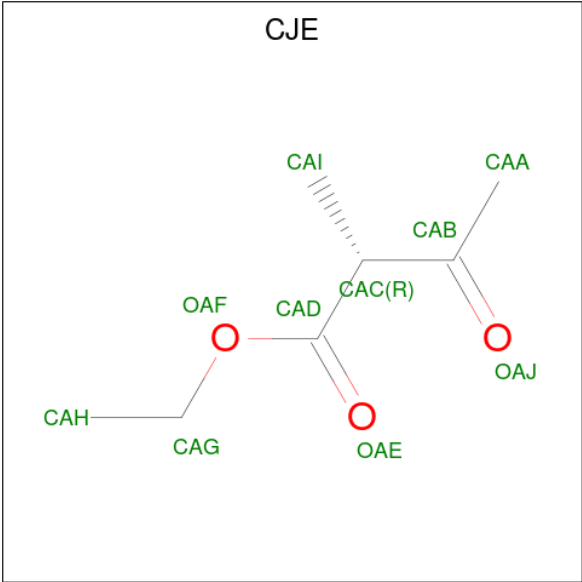
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	B	3	Total	Ca	0	0
			3	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is ethyl (2 {R})-2-methyl-3-oxidanylidene-butanoate (CCD ID: CJE) (formula: $C_7H_{12}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	7	3		

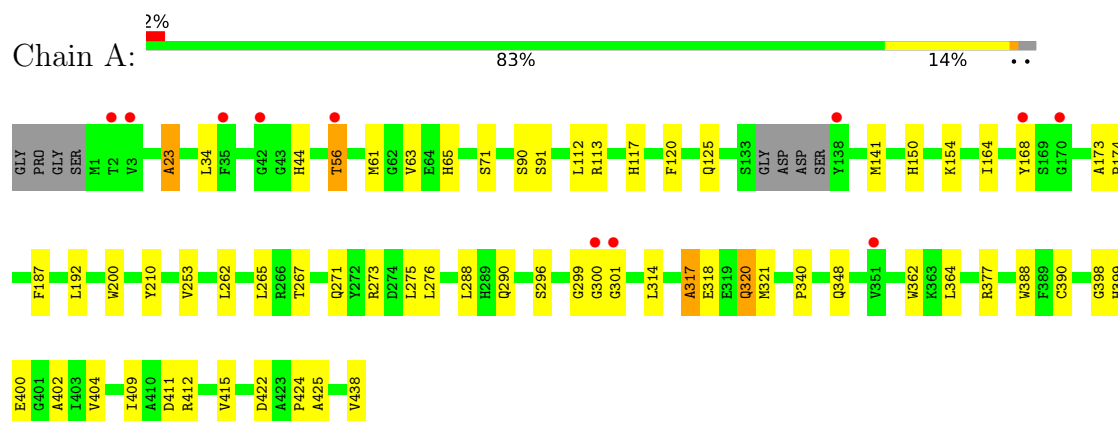
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	89	Total	O	0	0
			89	89		
8	B	92	Total	O	0	0
			92	92		

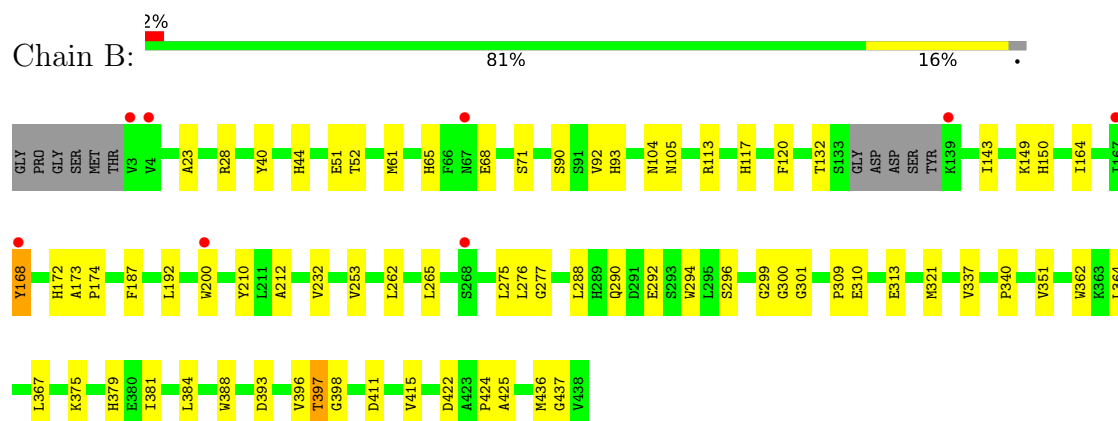
3 Residue-property plots

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: Amine oxidase LkcE



• Molecule 1: Amine oxidase LkcE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.50Å 125.50Å 156.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 2.80 48.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.98-2.80) 99.9 (48.98-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.237 , 0.256 0.226 , 0.255	Depositor DCC
R_{free} test set	1848 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	82.2	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7225	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: FAD, CJ8, CA, ACT, CJE, 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	0.72	0/3520	1.33	17/4772 (0.4%)
1	B	0.74	0/3508	1.37	22/4757 (0.5%)
All	All	0.73	0/7028	1.35	39/9529 (0.4%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	PRO	CA-C-N	7.33	130.44	120.54
1	B	309	PRO	C-N-CA	7.33	130.44	120.54
1	B	277	GLY	CA-C-N	6.65	132.27	122.82
1	B	277	GLY	C-N-CA	6.65	132.27	122.82
1	A	275	LEU	N-CA-C	6.48	118.42	111.36
1	B	104	ASN	CA-C-N	6.40	129.37	120.29
1	B	104	ASN	C-N-CA	6.40	129.37	120.29
1	A	56	THR	CB-CA-C	6.38	120.52	110.19
1	B	436	MET	CA-C-O	-6.06	114.50	121.47
1	A	23	ALA	CA-C-N	5.88	128.44	120.38
1	A	23	ALA	C-N-CA	5.88	128.44	120.38
1	A	174	PRO	N-CA-C	-5.87	104.56	112.48
1	A	173	ALA	N-CA-C	5.78	116.98	109.64
1	B	23	ALA	CA-C-N	5.68	128.16	120.38
1	B	23	ALA	C-N-CA	5.68	128.16	120.38
1	A	271	GLN	N-CA-C	-5.67	105.18	111.36
1	B	173	ALA	N-CA-C	5.64	116.80	109.64
1	B	310	GLU	N-CA-C	5.54	117.76	111.11
1	A	301	GLY	N-CA-C	-5.50	107.69	113.58
1	B	174	PRO	N-CA-C	-5.44	105.14	112.48
1	B	301	GLY	N-CA-C	-5.44	107.76	113.58
1	A	320	GLN	N-CA-C	5.34	118.38	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ALA	CA-C-N	5.23	127.29	120.28
1	A	317	ALA	C-N-CA	5.23	127.29	120.28
1	B	187	PHE	CA-C-N	5.22	127.54	120.38
1	B	187	PHE	C-N-CA	5.22	127.54	120.38
1	B	232	VAL	N-CA-C	5.22	113.32	108.15
1	A	398	GLY	CA-C-N	5.22	127.53	120.38
1	A	398	GLY	C-N-CA	5.22	127.53	120.38
1	A	120	PHE	CA-C-N	5.21	127.21	120.44
1	A	120	PHE	C-N-CA	5.21	127.21	120.44
1	A	187	PHE	CA-C-N	5.18	127.47	120.38
1	A	187	PHE	C-N-CA	5.18	127.47	120.38
1	B	120	PHE	CA-C-N	5.11	127.43	120.54
1	B	120	PHE	C-N-CA	5.11	127.43	120.54
1	B	143	ILE	CA-C-N	5.10	125.76	119.99
1	B	143	ILE	C-N-CA	5.10	125.76	119.99
1	B	398	GLY	CA-C-N	5.03	127.27	120.38
1	B	398	GLY	C-N-CA	5.03	127.27	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3431	0	3309	48	0
1	B	3418	0	3290	47	0
2	A	53	0	31	4	0
2	B	53	0	31	1	0
3	A	4	0	3	0	0
3	B	12	0	9	2	0
4	A	16	0	0	2	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
6	A	6	0	8	0	0
6	B	36	0	48	8	0
7	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	89	0	0	1	0
8	B	92	0	0	0	0
All	All	7225	0	6729	93	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 7.

All (93) 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:390:CYS:HB3	1:A:409:ILE:CD1	1.47	1.43
1:B:379:HIS:CB	1:B:437:GLY:HA3	1.72	1.19
1:A:390:CYS:HB3	1:A:409:ILE:HD12	1.31	1.12
1:B:379:HIS:HB3	1:B:437:GLY:HA3	1.29	1.07
1:A:390:CYS:HB3	1:A:409:ILE:HD11	1.47	0.95
1:B:379:HIS:HB3	1:B:437:GLY:CA	1.96	0.94
1:A:390:CYS:CB	1:A:409:ILE:CD1	2.44	0.92
1:B:379:HIS:HB2	1:B:437:GLY:HA3	1.50	0.90
1:A:400:GLU:O	1:A:404:VAL:HG23	1.76	0.85
1:A:321:MET:HB3	1:A:348:GLN:HG3	1.62	0.80
1:A:390:CYS:HB3	1:A:409:ILE:HD13	1.62	0.79
1:A:402:ALA:CB	2:A:601:FAD:H5'2	2.12	0.78
1:A:424:PRO:HD3	1:B:132:THR:HG21	1.65	0.77
1:A:273:ARG:HD2	1:A:273:ARG:O	1.85	0.77
1:A:390:CYS:CB	1:A:409:ILE:HD12	2.10	0.76
1:B:28:ARG:HH22	6:B:614:GOL:H32	1.51	0.75
1:B:379:HIS:CB	1:B:437:GLY:CA	2.59	0.75
6:B:609:GOL:H11	6:B:611:GOL:H12	1.73	0.71
1:B:90:SER:HB3	1:B:200[B]:TRP:HD1	1.59	0.68
1:A:168:TYR:O	4:A:603:CJ8:CAA	2.44	0.64
1:B:149:LYS:HG3	1:B:150:HIS:CD2	2.33	0.63
1:B:93:HIS:CD2	1:B:299:GLY:HA2	2.35	0.61
1:B:172:HIS:CE1	1:B:321:MET:HE1	2.36	0.61
1:B:92:VAL:H	1:B:105:ASN:HB2	1.66	0.61
1:B:90:SER:HB3	1:B:200[A]:TRP:CE3	2.36	0.61
6:B:609:GOL:H11	6:B:611:GOL:C1	2.31	0.60
1:A:412:ARG:HH11	1:A:412:ARG:HG3	1.67	0.60
1:B:262:LEU:HD13	1:B:276:LEU:HB2	1.84	0.59
1:B:40:TYR:HB2	6:B:611:GOL:H11	1.85	0.59
1:B:90:SER:HB3	1:B:200[B]:TRP:CD1	2.38	0.59
1:A:63:VAL:HG11	1:A:399:HIS:ND1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:HD2	1:A:117:HIS:ND1	2.19	0.57
1:B:51:GLU:H	3:B:603:ACT:H3	1.70	0.57
1:A:262:LEU:HD13	1:A:276:LEU:HB2	1.87	0.56
1:A:424:PRO:CD	1:B:132:THR:HG21	2.33	0.55
1:B:294:TRP:NE1	1:B:351:VAL:HG22	2.21	0.54
1:A:402:ALA:HB2	2:A:601:FAD:H5'2	1.91	0.52
1:A:23:ALA:HB2	1:A:34:LEU:HD13	1.91	0.51
1:A:273:ARG:HD2	1:A:273:ARG:C	2.35	0.51
1:A:90:SER:HB3	1:A:200:TRP:HD1	1.75	0.50
1:A:265:LEU:CD2	1:A:267:THR:HG22	2.42	0.50
1:B:113:ARG:HD2	1:B:117:HIS:HD2	1.77	0.49
1:B:375:LYS:HG2	1:B:393:ASP:O	2.12	0.49
1:B:296:SER:HB3	1:B:299:GLY:HA3	1.95	0.49
1:A:90:SER:HB3	1:A:200:TRP:CD1	2.48	0.49
1:A:164:ILE:HG12	1:A:192:LEU:HD22	1.95	0.49
1:A:422:ASP:OD1	1:A:424:PRO:HD2	2.13	0.48
1:A:412:ARG:HG3	1:A:412:ARG:NH1	2.28	0.48
1:A:424:PRO:CG	1:B:132:THR:HG21	2.44	0.48
6:B:609:GOL:H31	6:B:611:GOL:H12	1.95	0.48
1:A:422:ASP:HB3	1:A:425:ALA:HB3	1.95	0.48
1:A:296:SER:HB3	1:A:299:GLY:HA3	1.96	0.47
1:B:422:ASP:HB3	1:B:425:ALA:HB3	1.95	0.47
1:B:164:ILE:HG12	1:B:192:LEU:HD22	1.95	0.47
1:A:154:LYS:HE2	1:A:314:LEU:O	2.14	0.47
1:B:364:LEU:HD21	2:B:601:FAD:C9	2.45	0.47
1:B:422:ASP:OD1	1:B:424:PRO:HD2	2.15	0.47
1:A:400:GLU:O	1:A:404:VAL:CG2	2.58	0.46
1:B:113:ARG:HD2	1:B:117:HIS:CD2	2.50	0.46
1:B:168:TYR:CD1	1:B:168:TYR:N	2.83	0.46
1:A:364:LEU:HD21	2:A:601:FAD:C9	2.46	0.46
1:A:253:VAL:HG22	1:A:388:TRP:HB2	1.98	0.45
1:B:292:GLU:HG3	1:B:340:PRO:HG3	1.99	0.45
1:B:40:TYR:HB2	6:B:611:GOL:C1	2.46	0.45
1:A:168:TYR:O	4:A:603:CJ8:CAC	2.65	0.45
1:A:390:CYS:CB	1:A:409:ILE:HD11	2.32	0.45
1:B:253:VAL:HG22	1:B:388:TRP:HB2	1.98	0.45
1:A:63:VAL:HA	2:A:601:FAD:C4X	2.47	0.45
1:B:52:THR:OG1	1:B:337:VAL:HG13	2.16	0.45
1:A:65:HIS:HB3	1:A:200:TRP:CE3	2.52	0.44
1:A:317:ALA:O	1:A:320:GLN:HB2	2.16	0.44
1:A:424:PRO:HD3	1:B:132:THR:CG2	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:MET:HE3	1:B:288:LEU:HB2	2.00	0.44
1:A:411:ASP:HA	1:A:415:VAL:O	2.17	0.44
1:B:65:HIS:CE1	1:B:200[A]:TRP:CE3	3.06	0.44
1:A:125:GLN:HA	1:B:68:GLU:OE2	2.18	0.44
1:B:265:LEU:HD12	1:B:265:LEU:HA	1.81	0.44
1:A:290:GLN:HG2	1:A:340:PRO:O	2.19	0.43
1:B:275:LEU:HD12	1:B:381:ILE:HG23	2.00	0.43
1:A:44:HIS:HD2	1:A:362:TRP:CD1	2.37	0.43
1:A:412:ARG:HD3	1:A:438:VAL:CG1	2.49	0.43
1:B:396:VAL:HA	3:B:602:ACT:H3	2.00	0.42
1:B:44:HIS:HD2	1:B:362:TRP:CD1	2.36	0.42
1:B:321:MET:HB3	1:B:321:MET:HE2	1.77	0.42
1:B:367:LEU:HD11	1:B:397:THR:HG21	2.01	0.42
1:A:61:MET:HE3	1:A:288:LEU:HB2	2.01	0.42
1:A:150:HIS:HD2	8:A:719:HOH:O	2.02	0.42
1:B:212:ALA:HA	6:B:611:GOL:C3	2.51	0.41
1:B:212:ALA:N	6:B:611:GOL:H31	2.36	0.41
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.92	0.41
1:A:318:GLU:H	1:A:318:GLU:CD	2.28	0.41
1:B:411:ASP:HA	1:B:415:VAL:O	2.21	0.40
1:B:290:GLN:HG2	1:B:340:PRO:O	2.21	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	A	430/442 (97%)	414 (96%)	15 (4%)	1 (0%)	43	72
1	B	428/442 (97%)	413 (96%)	13 (3%)	2 (0%)	24	55
All	All	858/884 (97%)	827 (96%)	28 (3%)	3 (0%)	30	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	GLY
1	B	300	GLY
1	B	313	GLU

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/372 (99%)	361 (98%)	6 (2%)	55	83
1	B	365/372 (98%)	360 (99%)	5 (1%)	59	85
All	All	732/744 (98%)	721 (98%)	11 (2%)	57	84

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	71	SER
1	A	91	SER
1	A	141	MET
1	A	210	TYR
1	A	377	ARG
1	B	71	SER
1	B	168	TYR
1	B	210	TYR
1	B	384	LEU
1	B	397	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	251	GLN
1	A	348	GLN

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Mol	Chain	Res	Type
1	B	117	HIS
1	B	125	GLN
1	B	150	HIS
1	B	428	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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	ACT	A	602	-	3,3,3	1.18	0	3,3,3	0.88	0
2	FAD	A	601	-	58,58,58	0.52	1 (1%)	85,89,89	0.93	5 (5%)
3	ACT	B	602	-	3,3,3	1.20	0	3,3,3	0.92	0
6	GOL	B	613	-	5,5,5	0.10	0	5,5,5	0.24	0
6	GOL	B	614	-	5,5,5	0.10	0	5,5,5	0.34	0
3	ACT	B	604	-	3,3,3	1.16	0	3,3,3	0.96	0
6	GOL	A	606	-	5,5,5	0.07	0	5,5,5	0.19	0
6	GOL	B	612	-	5,5,5	0.15	0	5,5,5	0.19	0
6	GOL	B	610	-	5,5,5	0.14	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	B	601	-	58,58,58	0.46	0	85,89,89	0.85	3 (3%)
4	CJ8	A	603	-	15,15,15	0.64	0	18,18,18	0.80	0
6	GOL	B	611	-	5,5,5	0.12	0	5,5,5	0.56	0
3	ACT	B	603	-	3,3,3	1.22	0	3,3,3	0.92	0
7	CJE	B	608	-	8,9,9	1.50	2 (25%)	9,11,11	1.25	1 (11%)
6	GOL	B	609	-	5,5,5	0.12	0	5,5,5	0.51	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	A	601	-	-	11/34/50/50	0/6/6/6
6	GOL	B	614	-	-	4/4/4/4	-
6	GOL	B	613	-	-	3/4/4/4	-
6	GOL	A	606	-	-	2/4/4/4	-
6	GOL	B	612	-	-	0/4/4/4	-
6	GOL	B	610	-	-	4/4/4/4	-
2	FAD	B	601	-	-	12/34/50/50	0/6/6/6
4	CJ8	A	603	-	-	13/20/20/20	-
6	GOL	B	611	-	-	2/4/4/4	-
7	CJE	B	608	-	-	2/11/11/11	-
6	GOL	B	609	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	608	CJE	OAF-CAD	2.37	1.38	1.33
7	B	608	CJE	CAC-CAD	2.34	1.55	1.51
2	A	601	FAD	C9A-N10	2.33	1.45	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4'-C3'-C2'	4.13	120.44	113.57
2	A	601	FAD	C4'-C3'-C2'	3.69	119.71	113.57
2	A	601	FAD	O5'-C5'-C4'	-3.46	100.13	109.36
7	B	608	CJE	CAB-CAC-CAD	2.69	115.69	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	O2P-P-O3P	2.48	113.97	107.27
2	B	601	FAD	O2P-P-O3P	2.47	113.96	107.27
2	A	601	FAD	C5X-C9A-N10	-2.43	115.77	117.97
2	B	601	FAD	O4'-C4'-C3'	2.24	114.50	109.25
2	A	601	FAD	O4'-C4'-C3'	-2.02	104.53	109.25

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'
2	A	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	C2'-C1'-N10-C10
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	N10-C1'-C2'-C3'
4	A	603	CJ8	CAE-CAF-CAG-OAP
4	A	603	CJ8	OAM-CAF-CAG-CAH
4	A	603	CJ8	CAF-CAG-CAH-OAO
4	A	603	CJ8	CAF-CAG-CAH-NAI
4	A	603	CJ8	OAP-CAG-CAH-OAO
4	A	603	CJ8	OAP-CAG-CAH-NAI
6	B	609	GOL	C1-C2-C3-O3
6	B	610	GOL	O1-C1-C2-C3
6	B	610	GOL	C1-C2-C3-O3
6	B	613	GOL	O1-C1-C2-O2
6	B	613	GOL	O1-C1-C2-C3
2	B	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-C5'
7	B	608	CJE	OAE-CAD-OAF-CAG
7	B	608	CJE	CAC-CAD-OAF-CAG
4	A	603	CJ8	OAM-CAF-CAG-OAP
6	B	614	GOL	O1-C1-C2-O2
2	B	601	FAD	O3'-C3'-C4'-O4'
6	A	606	GOL	C1-C2-C3-O3
6	B	611	GOL	C1-C2-C3-O3
6	B	614	GOL	O1-C1-C2-C3
6	B	614	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	606	GOL	O2-C2-C3-O3
6	B	609	GOL	O2-C2-C3-O3
6	B	610	GOL	O1-C1-C2-O2
6	B	610	GOL	O2-C2-C3-O3
2	B	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	O4B-C4B-C5B-O5B
6	B	613	GOL	C1-C2-C3-O3
2	A	601	FAD	C2B-C1B-N9A-C8A
2	B	601	FAD	C2B-C1B-N9A-C8A
2	A	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	C5B-O5B-PA-O3P
4	A	603	CJ8	CAE-CAF-CAG-CAH
6	B	611	GOL	O2-C2-C3-O3
4	A	603	CJ8	OAN-CAE-CAF-CAG
4	A	603	CJ8	NAD-CAE-CAF-CAG
2	B	601	FAD	C3B-C4B-C5B-O5B
4	A	603	CJ8	CAC-CAA-CAB-NAD
6	B	614	GOL	O2-C2-C3-O3
4	A	603	CJ8	OAN-CAE-CAF-OAM
4	A	603	CJ8	NAD-CAE-CAF-OAM
2	A	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	O4B-C1B-N9A-C8A
2	B	601	FAD	O4B-C1B-N9A-C8A

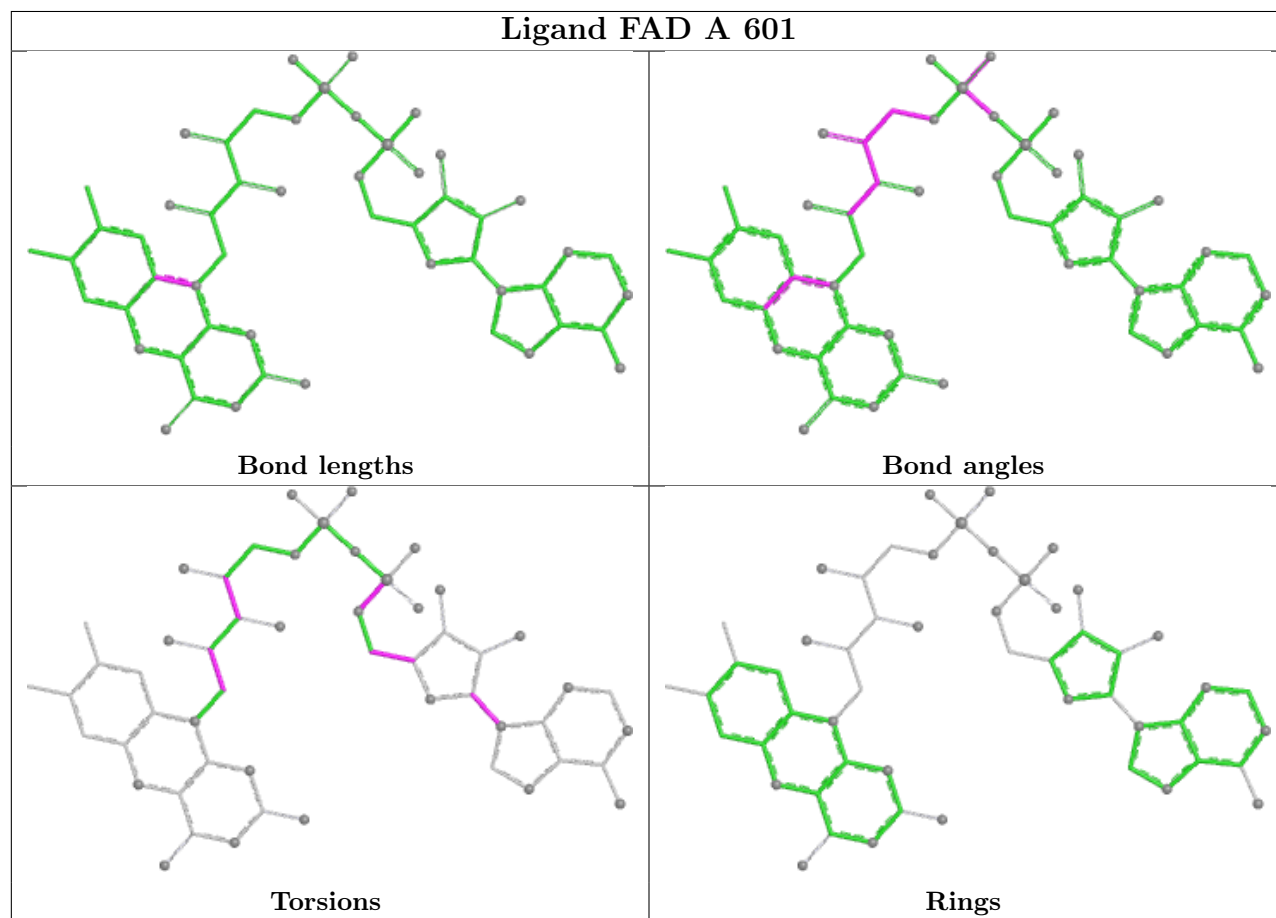
There are no ring outliers.

8 monomers are involved in 17 short contacts:

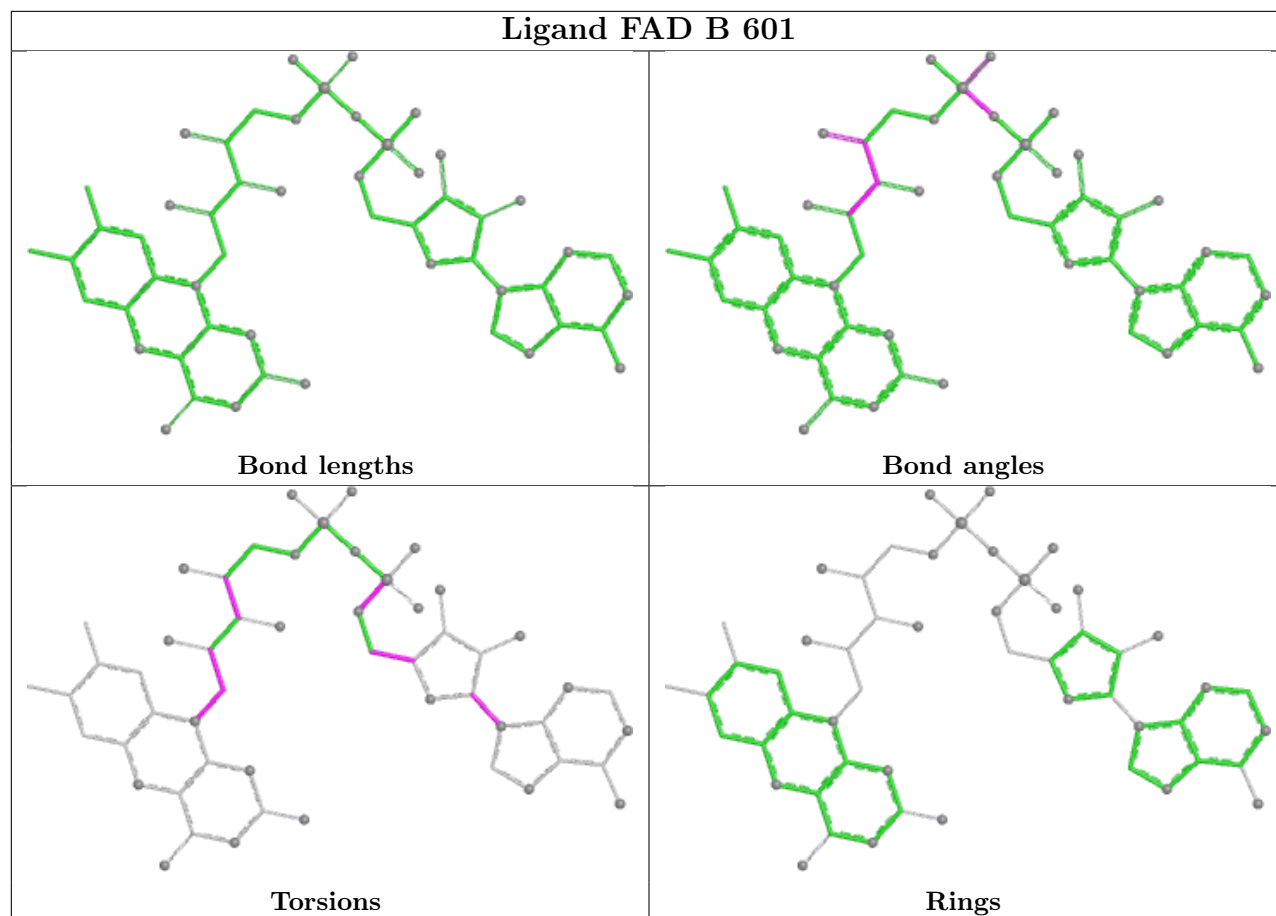
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	4	0
3	B	602	ACT	1	0
6	B	614	GOL	1	0
2	B	601	FAD	1	0
4	A	603	CJ8	2	0
6	B	611	GOL	7	0
3	B	603	ACT	1	0
6	B	609	GOL	3	0

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.

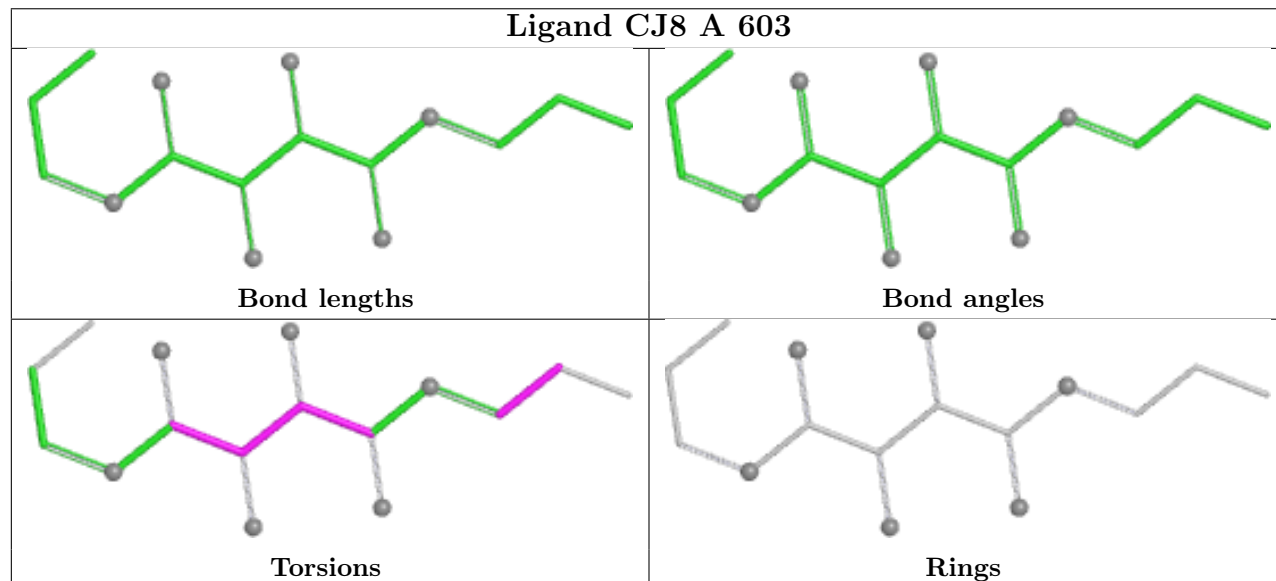
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

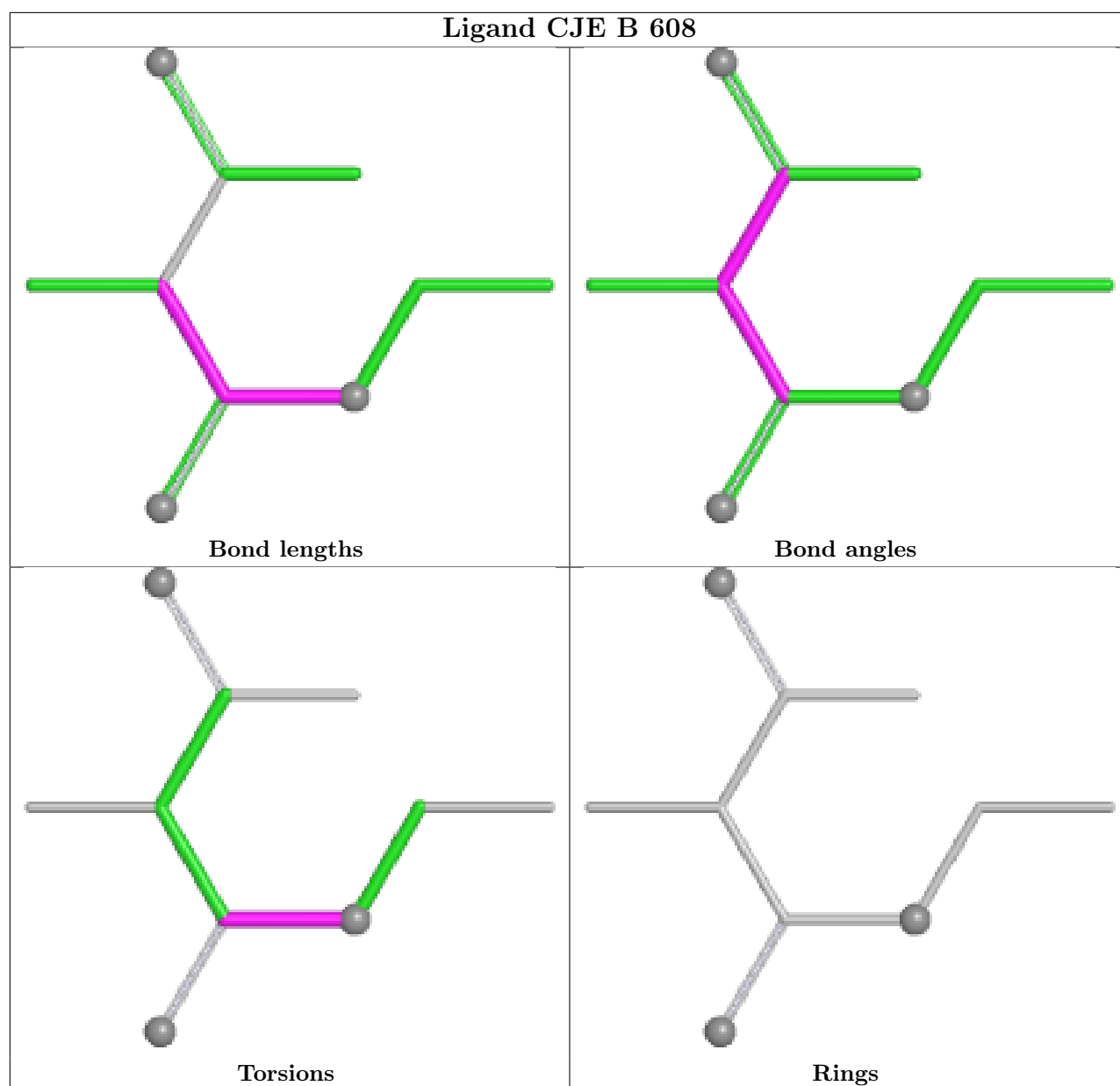


Ligand FAD B 601



Ligand CJ8 A 603





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	434/442 (98%)	0.42	11 (2%) 58 48	56, 87, 123, 152	0
1	B	431/442 (97%)	0.34	8 (1%) 66 57	33, 82, 115, 144	1 (0%)
All	All	865/884 (97%)	0.38	19 (2%) 62 52	33, 85, 119, 152	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	LYS	4.0
1	B	3	VAL	3.6
1	B	200[A]	TRP	3.4
1	A	56	THR	3.1
1	A	2	THR	2.7
1	B	168	TYR	2.7
1	B	4	VAL	2.6
1	A	3	VAL	2.5
1	A	138	TYR	2.5
1	A	168	TYR	2.4
1	A	42	GLY	2.3
1	B	67	ASN	2.2
1	B	167	ILE	2.2
1	A	35	PHE	2.2
1	A	301	GLY	2.2
1	A	300	GLY	2.1
1	A	351	VAL	2.1
1	A	170	GLY	2.1
1	B	268	SER	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

There are no oligosaccharides in this entry.

6.4 Ligands

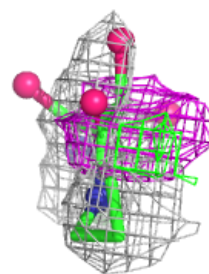
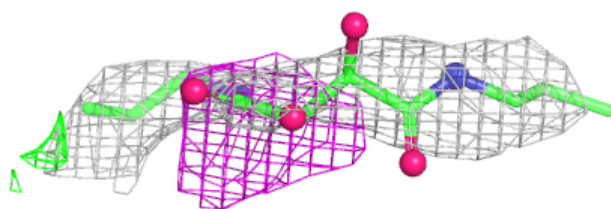
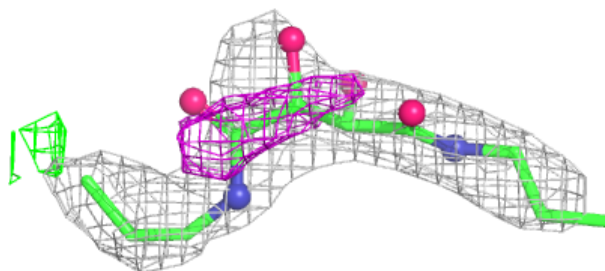
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACT	A	602	4/4	0.18	0.24	78,80,80,80	0
5	CA	A	604	1/1	0.58	0.29	159,159,159,159	1
3	ACT	B	603	4/4	0.70	0.20	93,94,95,95	0
3	ACT	B	604	4/4	0.71	0.24	102,102,102,102	0
5	CA	B	607	1/1	0.77	0.29	130,130,130,130	0
6	GOL	B	609	6/6	0.79	0.18	97,98,99,99	0
6	GOL	B	612	6/6	0.79	0.12	105,106,107,107	0
6	GOL	B	610	6/6	0.81	0.19	100,101,102,102	0
6	GOL	B	613	6/6	0.82	0.13	112,113,113,113	0
6	GOL	B	614	6/6	0.82	0.16	98,98,98,98	6
4	CJ8	A	603	16/16	0.83	0.27	100,112,116,117	0
6	GOL	A	606	6/6	0.85	0.21	118,120,120,120	0
7	CJE	B	608	10/10	0.86	0.28	108,109,111,111	0
6	GOL	B	611	6/6	0.88	0.17	116,118,118,119	0
3	ACT	B	602	4/4	0.89	0.17	86,86,87,90	0
5	CA	A	605	1/1	0.89	0.30	109,109,109,109	0
5	CA	B	606	1/1	0.89	0.19	117,117,117,117	0
2	FAD	A	601	53/53	0.93	0.10	75,86,100,102	0
5	CA	B	605	1/1	0.93	0.19	127,127,127,127	0
2	FAD	B	601	53/53	0.94	0.09	77,83,91,92	0

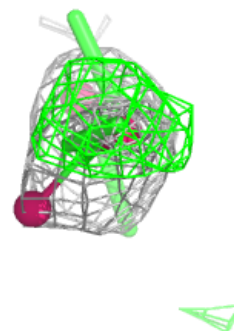
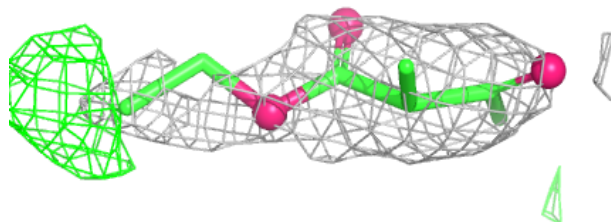
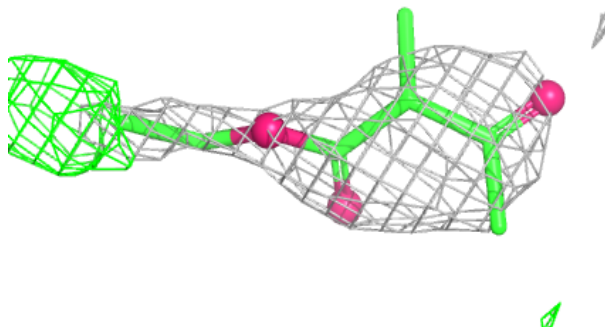
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CJ8 A 603:

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

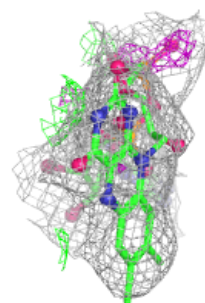
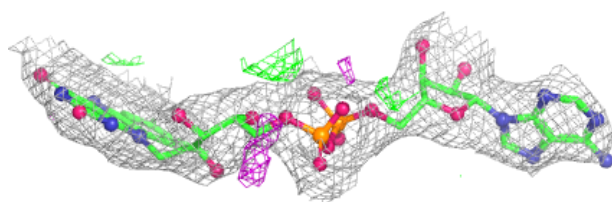
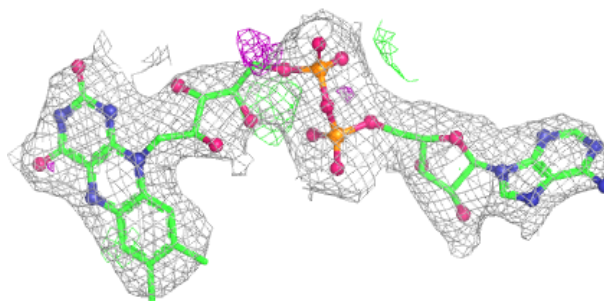
**Electron density around CJE B 608:**

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

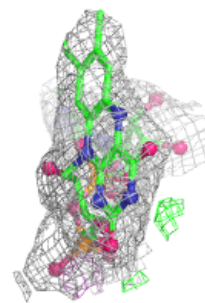
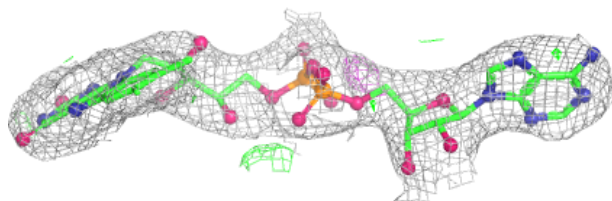
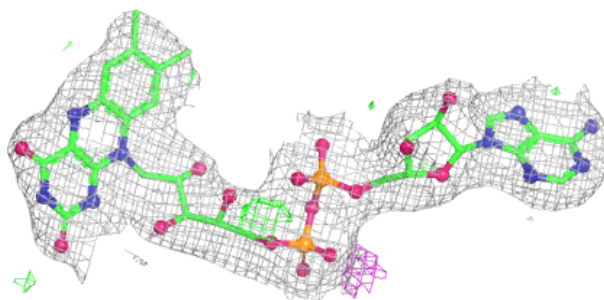


Electron density around FAD A 601:

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

**Electron density around FAD 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.