



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:32 am BST

PDB ID : 6F32
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 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 : 2.11
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) : 2.11

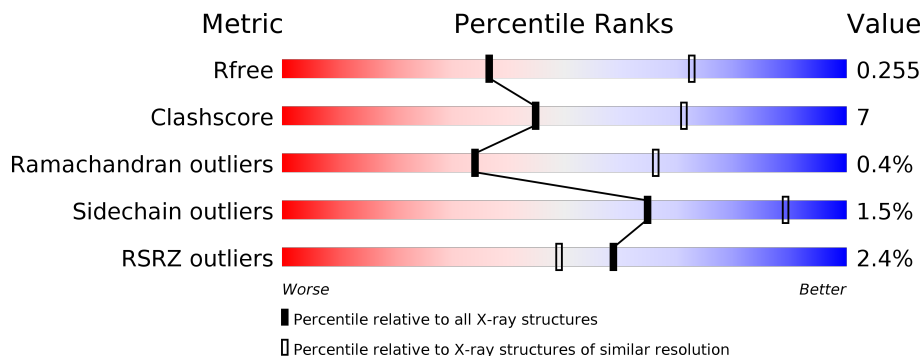
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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	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
4	CJ8	A	603	-	-	-	X
5	CA	A	605	-	-	-	X
5	CA	B	605	-	-	-	X
6	GOL	A	606	-	-	-	X
6	GOL	B	610	-	-	-	X
6	GOL	B	611	-	-	X	-
6	GOL	B	613	-	-	-	X
6	GOL	B	614	-	-	-	X

2 Entry composition [i](#)

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.

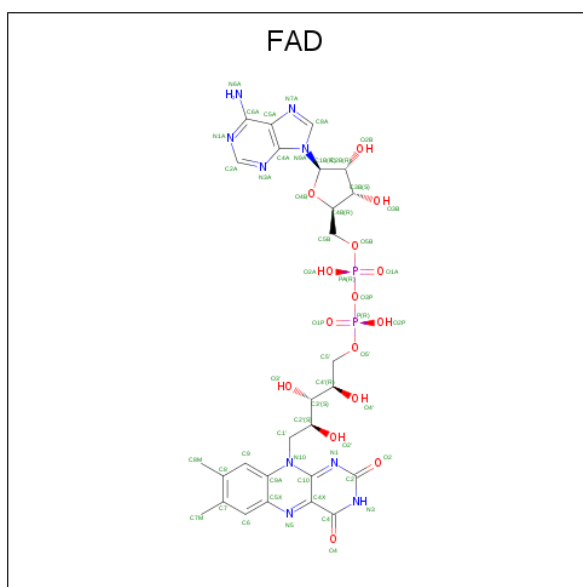
- Molecule 1 is a protein called Amine oxidase LkcE.

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

There are 12 discrepancies between the modelled and reference sequences:

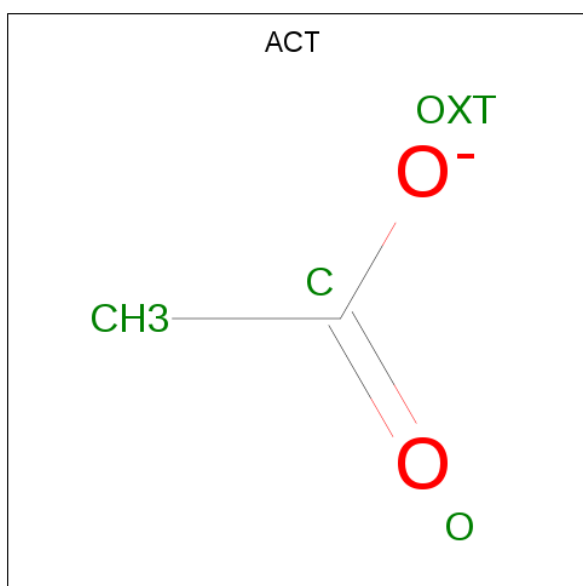
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q83X90
A	-2	PRO	-	expression tag	UNP Q83X90
A	-1	GLY	-	expression tag	UNP Q83X90
A	0	SER	-	expression tag	UNP Q83X90
A	54	GLN	ARG	conflict	UNP Q83X90
A	424	PRO	LEU	conflict	UNP Q83X90
B	-3	GLY	-	expression tag	UNP Q83X90
B	-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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



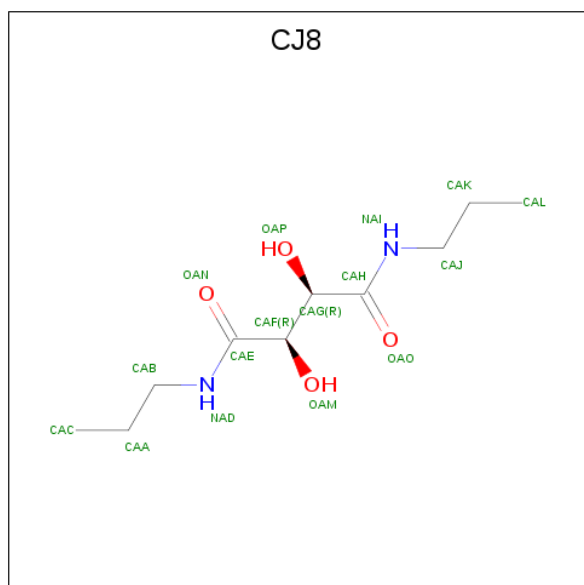
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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 (three-letter code: CJ8) (formula: C₁₀H₂₀N₂O₄) (labeled as "Ligand of Interest" by author).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

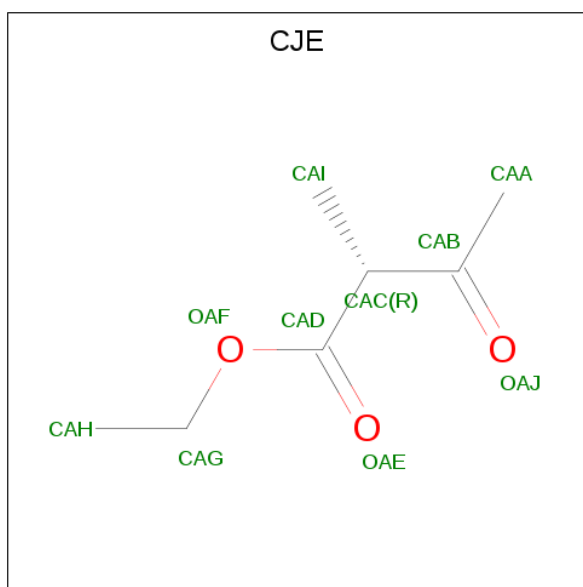
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Ca	0	0
			3	3		
5	A	2	Total	Ca	0	0
			2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is ethyl (2 {R})-2-methyl-3-oxidanylidene-butanoate (three-letter code: CJE) (formula: C₇H₁₂O₃) (labeled as "Ligand of Interest" by author).



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

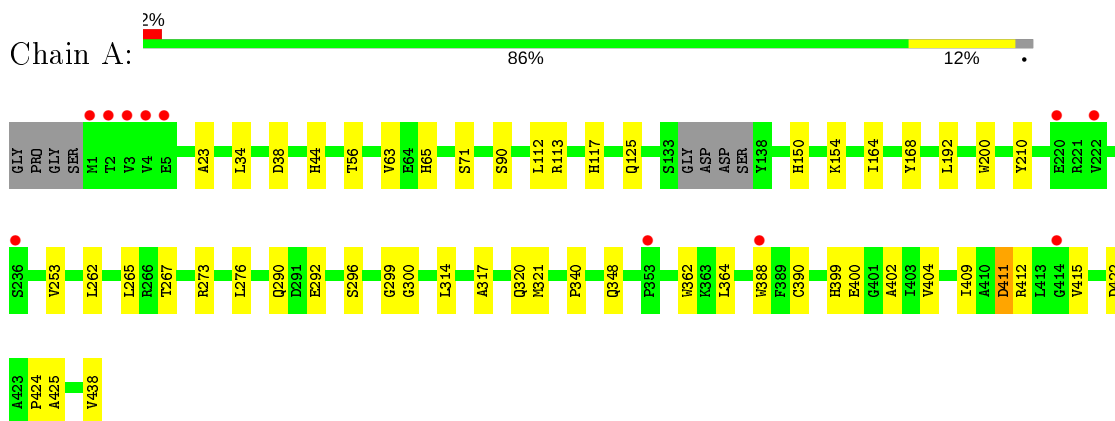
- Molecule 8 is water.

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

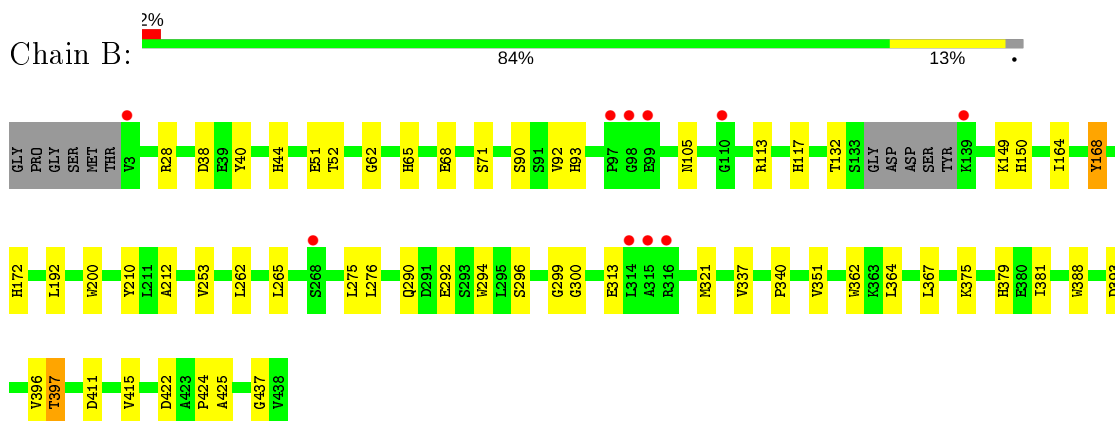
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.98-2.80) 99.9 (48.98-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.65Å)	Xtrriage
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	Xtrriage
Anisotropy	0.081	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7225	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage'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: GOL, CA, CJE, CJ8, ACT, FAD

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	0.42	0/3520	0.67	0/4772
1	B	0.43	0/3508	0.69	0/4757
All	All	0.43	0/7028	0.68	0/9529

There are no bond length outliers.

There are no bond angle outliers.

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	3431	0	3309	46	0
1	B	3418	0	3290	46	0
2	A	53	0	31	4	0
2	B	53	0	31	2	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	10	0	0	0	0
8	A	89	0	0	1	0
8	B	92	0	0	0	0
All	All	7225	0	6729	90	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 (90) 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:O	1:A:273:ARG:HD2	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: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:HG3	1:A:412:ARG:HH11	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:113:ARG:HD2	1:A:117:HIS:ND1	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:HG11	1:A:399: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: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:62:GLY:HA2	2:B:601:FAD:HM72	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:N	1:B:168:TYR:CD1	2.83	0.46
1:A:273:ARG:C	1:A:273:ARG:HD2	2.35	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:317:ALA:O	1:A:320:GLN:HB2	2.16	0.44
1:A:65:HIS:HB3	1:A:200:TRP:CE3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:PRO:HD3	1:B:132:THR:CG2	2.40	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:B:265:LEU:HA	1:B:265:LEU:HD12	1.81	0.44
1:A:125:GLN:HA	1:B:68:GLU:OE2	2.18	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:367:LEU:HD11	1:B:397:THR:HG21	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:B:172:HIS:CE1	1:B:321:MET:HE3	2.56	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 [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	430/442 (97%)	414 (96%)	15 (4%)	1 (0%)	47	78
1	B	428/442 (97%)	413 (96%)	13 (3%)	2 (0%)	29	61
All	All	858/884 (97%)	827 (96%)	28 (3%)	3 (0%)	34	72

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 [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	367/372 (99%)	361 (98%)	6 (2%)	62	88
1	B	365/372 (98%)	360 (99%)	5 (1%)	67	90
All	All	732/744 (98%)	721 (98%)	11 (2%)	65	89

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

Mol	Chain	Res	Type
1	A	38	ASP
1	A	56	THR
1	A	71	SER
1	A	210	TYR
1	A	292	GLU
1	A	411	ASP
1	B	38	ASP
1	B	71	SER
1	B	168	TYR
1	B	210	TYR
1	B	397	THR

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

Mol	Chain	Res	Type
1	A	179	ASN
1	A	251	GLN
1	B	93	HIS
1	B	105	ASN
1	B	150	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	172	HIS
1	B	179	ASN

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 carbohydrates 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	B	603	-	1,3,3	5.36	1 (100%)	0,3,3	0.00	-
2	FAD	B	601	-	51,58,58	1.51	5 (9%)	60,89,89	2.39	11 (18%)
2	FAD	A	601	-	51,58,58	1.57	4 (7%)	60,89,89	2.44	12 (20%)
3	ACT	B	604	-	1,3,3	4.68	1 (100%)	0,3,3	0.00	-
4	CJ8	A	603	-	15,15,15	0.64	0	18,18,18	0.79	0
3	ACT	A	602	-	1,3,3	5.30	1 (100%)	0,3,3	0.00	-
6	GOL	A	606	-	5,5,5	0.06	0	5,5,5	0.20	0
6	GOL	B	612	-	5,5,5	0.14	0	5,5,5	0.21	0
6	GOL	B	611	-	5,5,5	0.11	0	5,5,5	0.53	0
6	GOL	B	609	-	5,5,5	0.10	0	5,5,5	0.48	0
6	GOL	B	613	-	5,5,5	0.09	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	B	602	-	1,3,3	5.08	1 (100%)	0,3,3	0.00	-
6	GOL	B	614	-	5,5,5	0.09	0	5,5,5	0.33	0
7	CJE	B	608	-	9,9,9	1.54	2 (22%)	10,11,11	1.27	1 (10%)
6	GOL	B	610	-	5,5,5	0.12	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
2	FAD	B	601	-	-	10/30/50/50	0/6/6/6
2	FAD	A	601	-	-	11/30/50/50	0/6/6/6
4	CJ8	A	603	-	-	13/20/20/20	-
6	GOL	A	606	-	-	2/4/4/4	-
6	GOL	B	612	-	-	0/4/4/4	-
6	GOL	B	611	-	-	2/4/4/4	-
6	GOL	B	609	-	-	2/4/4/4	-
6	GOL	B	613	-	-	3/4/4/4	-
6	GOL	B	614	-	-	4/4/4/4	-
7	CJE	B	608	-	-	2/11/11/11	-
6	GOL	B	610	-	-	4/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4X-C10	7.52	1.46	1.38
2	B	601	FAD	C4X-C10	7.33	1.46	1.38
3	B	603	ACT	CH3-C	5.36	1.55	1.48
3	A	602	ACT	CH3-C	5.30	1.55	1.48
3	B	602	ACT	CH3-C	5.08	1.55	1.48
2	A	601	FAD	C9A-N10	4.94	1.45	1.38
3	B	604	ACT	CH3-C	4.68	1.54	1.48
2	B	601	FAD	C9A-N10	4.11	1.44	1.38
2	A	601	FAD	C4-N3	3.48	1.39	1.33
2	A	601	FAD	C4-C4X	3.36	1.47	1.41
2	B	601	FAD	C4-N3	3.33	1.38	1.33
2	B	601	FAD	C4-C4X	3.28	1.47	1.41
7	B	608	CJE	OAF-CAD	2.41	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C5X-N5	2.38	1.39	1.35
7	B	608	CJE	CAC-CAD	2.25	1.55	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4-N3-C2	12.76	125.92	115.14
2	A	601	FAD	C4-N3-C2	12.71	125.87	115.14
2	B	601	FAD	C4X-C4-N3	-6.82	114.11	123.43
2	A	601	FAD	C4X-C4-N3	-6.59	114.42	123.43
2	B	601	FAD	C1'-N10-C9A	5.16	122.35	118.29
2	A	601	FAD	C1'-N10-C9A	5.09	122.30	118.29
2	B	601	FAD	C10-C4X-N5	4.64	124.47	121.26
2	A	601	FAD	C10-C4X-N5	4.63	124.46	121.26
2	B	601	FAD	C4-C4X-C10	-4.00	117.30	119.95
2	A	601	FAD	C4-C4X-C10	-3.73	117.48	119.95
2	A	601	FAD	C4X-C10-N10	-3.68	116.52	120.30
2	B	601	FAD	C4X-C10-N10	-3.49	116.72	120.30
2	A	601	FAD	O5'-C5'-C4'	-3.46	100.13	109.36
2	B	601	FAD	C4'-C3'-C2'	3.40	120.44	113.36
2	A	601	FAD	C1'-N10-C10	-3.20	115.54	118.41
2	A	601	FAD	C4'-C3'-C2'	3.05	119.71	113.36
7	B	608	CJE	OAF-CAD-CAC	2.85	113.71	111.26
2	A	601	FAD	C5X-C9A-N10	-2.69	115.77	117.72
2	B	601	FAD	C1'-N10-C10	-2.68	116.01	118.41
2	B	601	FAD	P-O3P-PA	-2.43	124.48	132.83
2	B	601	FAD	O4'-C4'-C3'	2.22	114.50	109.10
2	A	601	FAD	P-O3P-PA	-2.21	125.24	132.83
2	B	601	FAD	C5A-C6A-N6A	2.14	123.61	120.35
2	A	601	FAD	C5A-C6A-N6A	2.11	123.55	120.35

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C2'-C1'-N10-C10
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	N10-C1'-C2'-C3'
2	A	601	FAD	C2'-C1'-N10-C10
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'
2	A	601	FAD	C2'-C3'-C4'-O4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	O3'-C3'-C4'-O4'
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	613	GOL	O1-C1-C2-O2
6	B	613	GOL	O1-C1-C2-C3
6	B	610	GOL	O1-C1-C2-C3
6	B	610	GOL	C1-C2-C3-O3
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C2'-C3'-C4'-O4'
7	B	608	CJE	OAE-CAD-OAF-CAG
2	B	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-C5'
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	A	601	FAD	O4B-C4B-C5B-O5B
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
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
4	A	603	CJ8	OAN-CAE-CAF-CAG
4	A	603	CJ8	NAD-CAE-CAF-CAG
2	B	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	C5B-O5B-PA-O3P
6	B	613	GOL	C1-C2-C3-O3
4	A	603	CJ8	CAE-CAF-CAG-CAH
6	B	611	GOL	O2-C2-C3-O3
2	B	601	FAD	C3B-C4B-C5B-O5B
4	A	603	CJ8	OAN-CAE-CAF-OAM
4	A	603	CJ8	CAC-CAA-CAB-NAD

Continued on next page...

Continued from previous page...

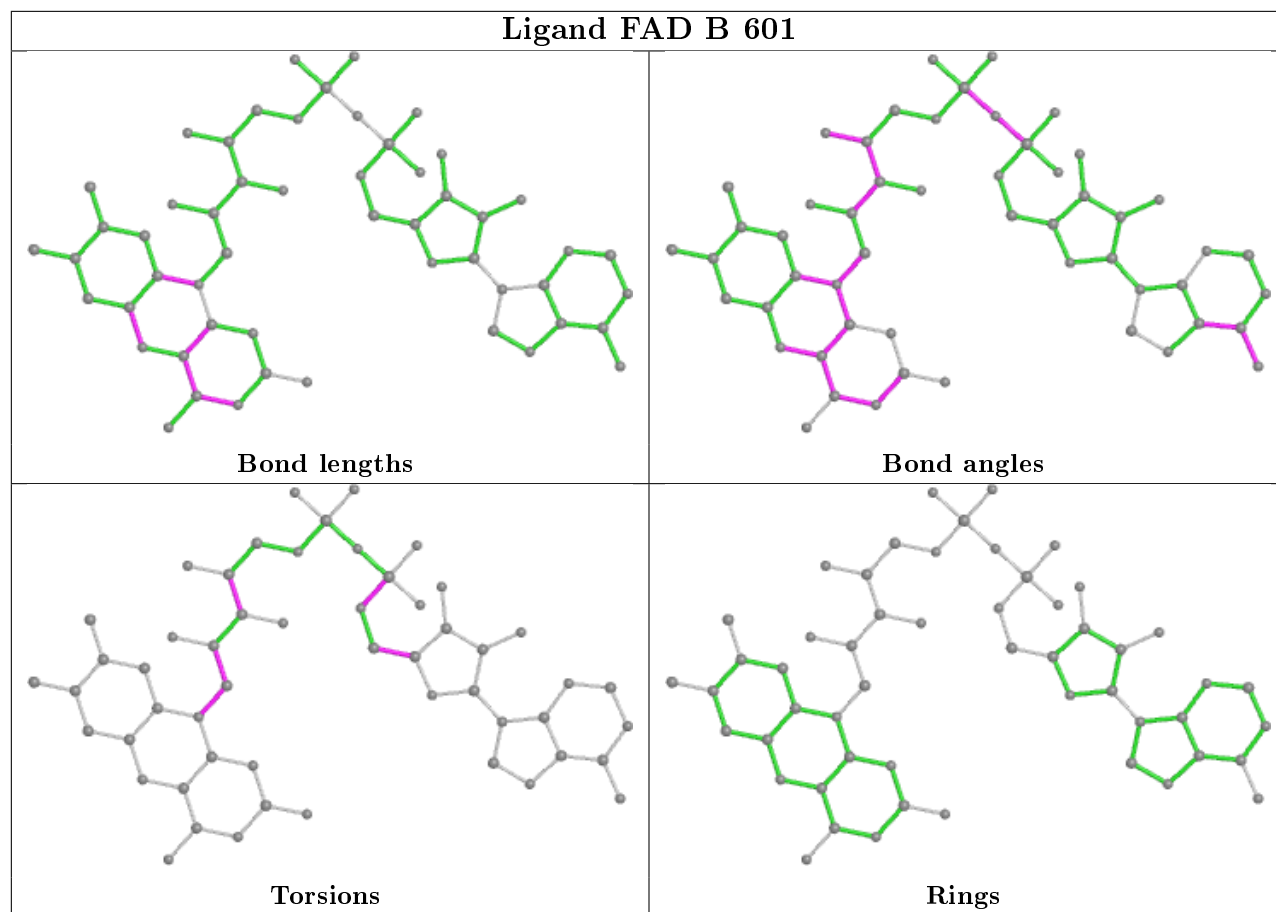
Mol	Chain	Res	Type	Atoms
4	A	603	CJ8	NAD-CAE-CAF-OAM
2	A	601	FAD	C3B-C4B-C5B-O5B
6	B	614	GOL	O2-C2-C3-O3
2	A	601	FAD	C5'-O5'-P-O1P

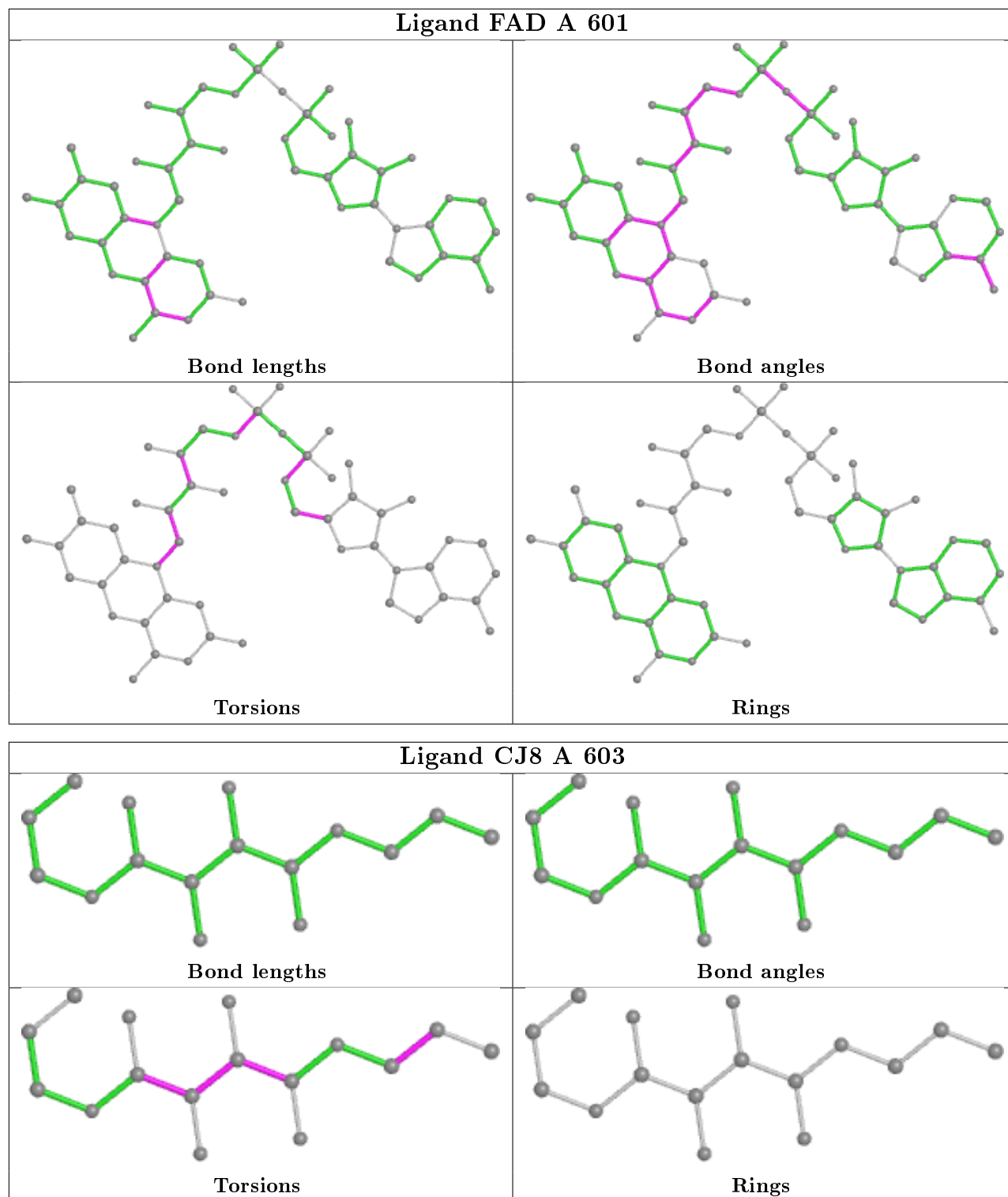
There are no ring outliers.

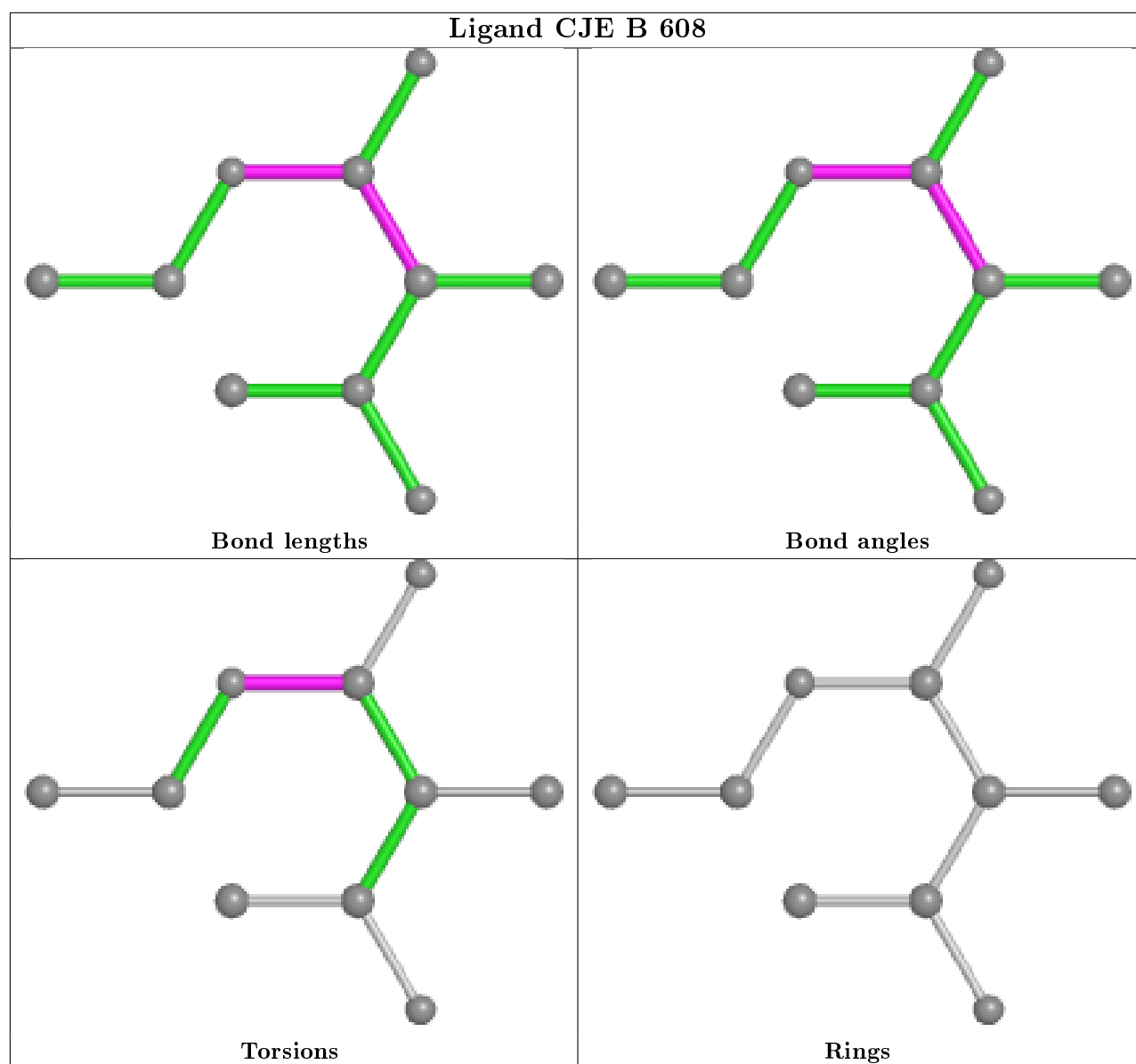
8 monomers are involved in 18 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	434/442 (98%)	0.27	11 (2%) 57 47	56, 87, 123, 152	0
1	B	431/442 (97%)	0.17	10 (2%) 60 51	59, 82, 115, 144	0
All	All	865/884 (97%)	0.22	21 (2%) 59 49	56, 85, 119, 152	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	SER	4.0
1	A	3	VAL	3.8
1	A	222	VAL	3.0
1	B	98	GLY	2.9
1	B	314	LEU	2.9
1	A	4	VAL	2.7
1	B	139	LYS	2.6
1	A	414	GLY	2.6
1	B	315	ALA	2.5
1	B	3	VAL	2.5
1	A	2	THR	2.5
1	B	97	PRO	2.3
1	B	316	ARG	2.3
1	A	5	GLU	2.3
1	A	1	MET	2.3
1	A	220	GLU	2.2
1	A	236	SER	2.2
1	B	110	GLY	2.1
1	A	353	PRO	2.1
1	B	99	GLU	2.1
1	A	388	TRP	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 carbohydrates in this entry.

6.4 Ligands [i](#)

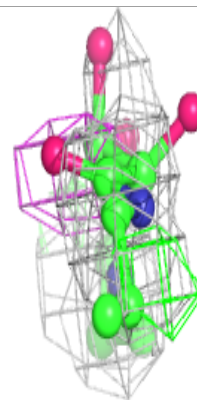
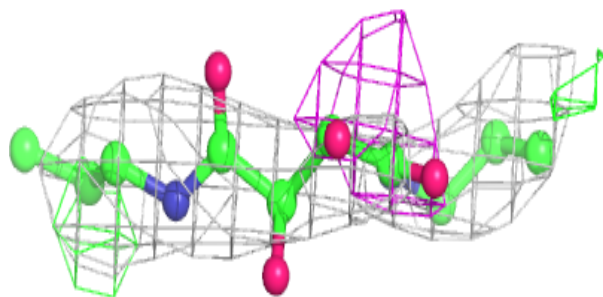
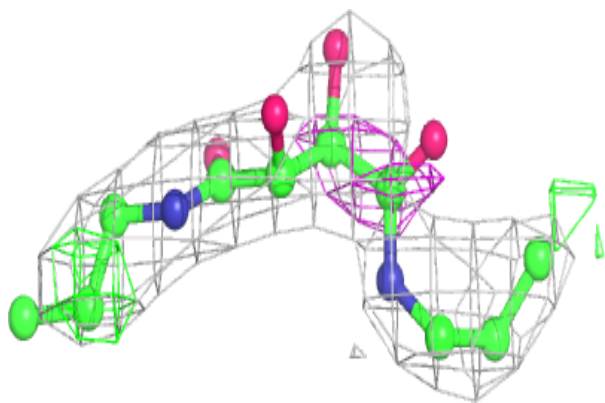
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	A	602	4/4	0.57	0.24	78,80,80,80	0
4	CJ8	A	603	16/16	0.66	0.46	100,112,116,117	0
3	ACT	B	603	4/4	0.66	0.30	93,94,95,95	0
5	CA	B	605	1/1	0.67	0.48	127,127,127,127	0
6	GOL	A	606	6/6	0.70	0.66	118,120,120,120	0
6	GOL	B	614	6/6	0.70	0.55	98,98,98,98	6
6	GOL	B	613	6/6	0.70	0.54	112,113,113,113	0
7	CJE	B	608	10/10	0.71	0.35	108,109,111,111	0
6	GOL	B	612	6/6	0.73	0.17	105,106,107,107	0
6	GOL	B	609	6/6	0.74	0.28	97,98,99,99	0
6	GOL	B	610	6/6	0.75	0.45	100,101,102,102	0
5	CA	A	605	1/1	0.77	0.62	109,109,109,109	0
6	GOL	B	611	6/6	0.78	0.35	116,118,118,119	0
5	CA	B	607	1/1	0.81	0.16	130,130,130,130	0
5	CA	B	606	1/1	0.84	0.17	117,117,117,117	0
5	CA	A	604	1/1	0.86	0.66	159,159,159,159	1
3	ACT	B	604	4/4	0.88	0.34	102,102,102,102	0
3	ACT	B	602	4/4	0.88	0.22	86,86,87,90	0
2	FAD	A	601	53/53	0.92	0.20	75,86,100,102	0
2	FAD	B	601	53/53	0.95	0.18	77,83,91,92	0

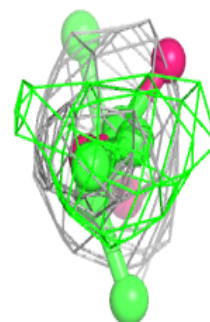
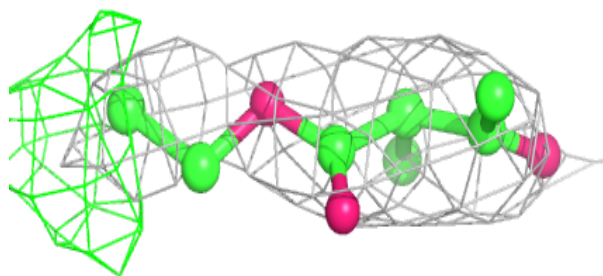
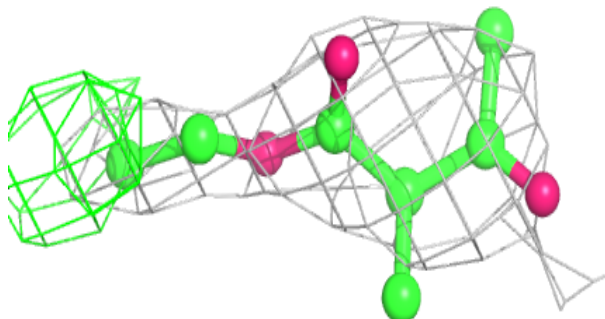
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

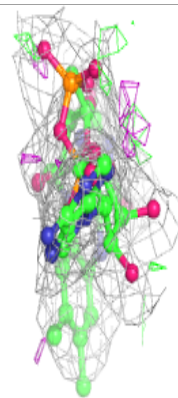
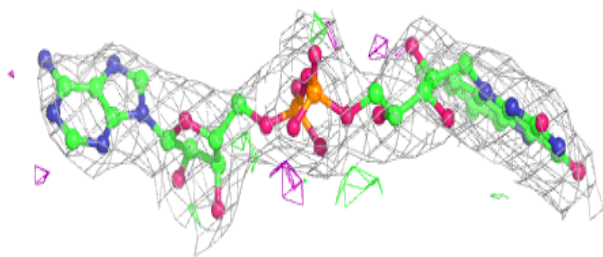
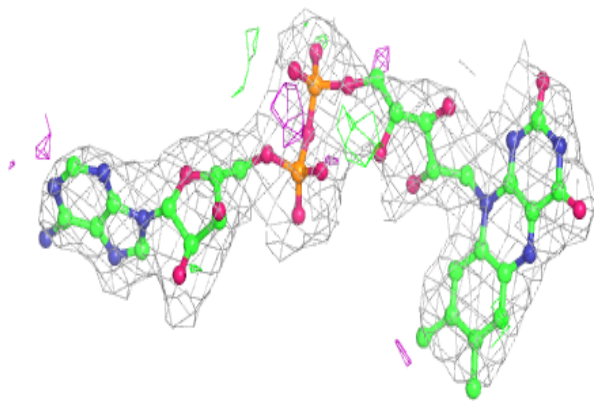
**Electron density around CJE B 608:**

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

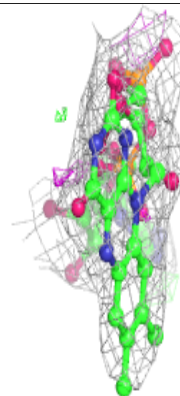
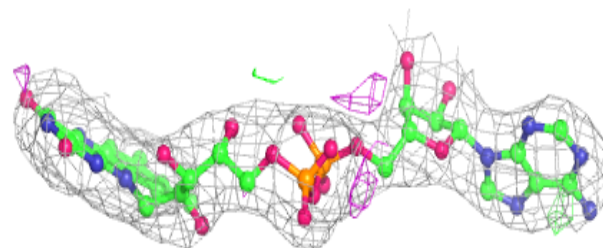
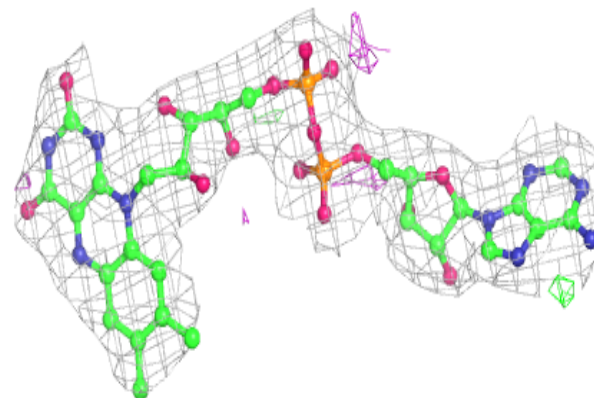


Electron density around FAD A 601:

$2mF_o-DF_c$ (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

There are no such residues in this entry.