



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:55 pm BST

PDB ID : 5BRT
Title : Crystal Structure of 2-hydroxybiphenyl 3-monooxygenase from *Pseudomonas azelaica* with 2-hydroxybiphenyl in the active site
Authors : Kanteev, M.; Bregman-Cohen, A.; Deri, B.; Adir, N.; Fishman, A.
Deposited on : 2015-06-01
Resolution : 2.30 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

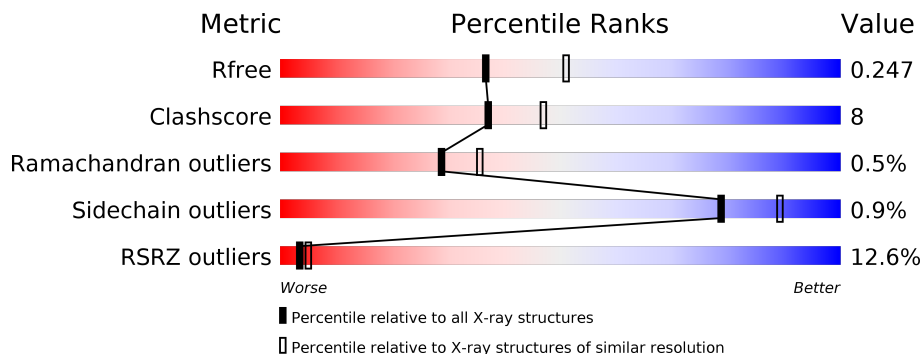
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	586	
1	B	586	

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
2	FAD	A	601	X	-	-	-
2	FAD	B	601	X	-	-	-

2 Entry composition [i](#)

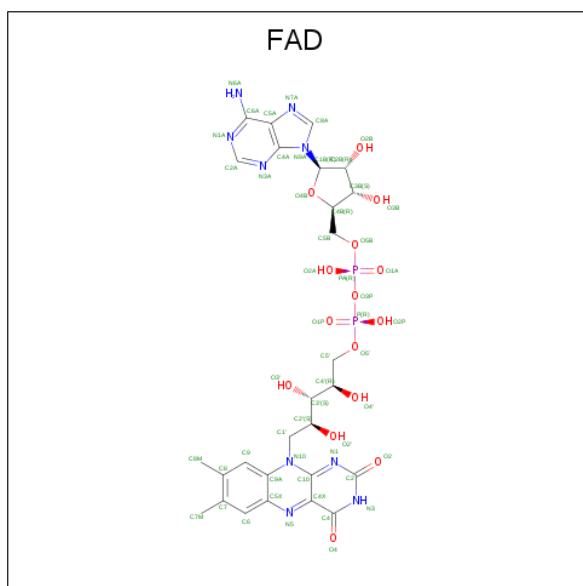
There are 4 unique types of molecules in this entry. The entry contains 9534 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-hydroxybiphenyl-3-monooxygenase.

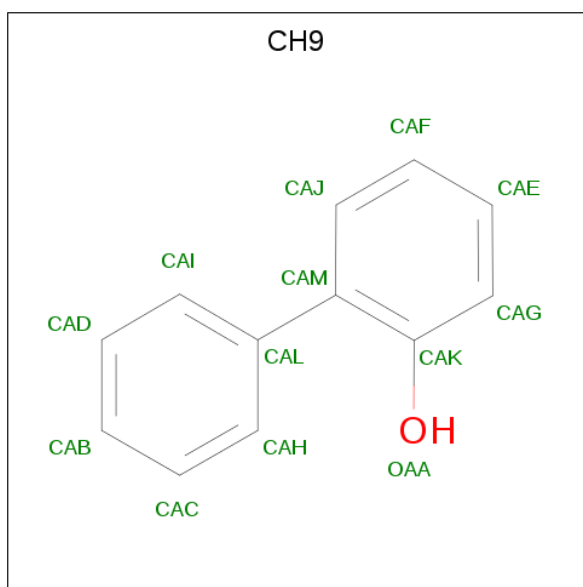
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	554	Total	C	N	O	S	0	0	0
			4258	2692	748	799	19			
1	B	559	Total	C	N	O	S	0	0	0
			4304	2720	757	807	20			

- 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
			Total	C	N	O	P		
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 2-HYDROXYBIPHENYL (three-letter code: CH9) (formula: $C_{12}H_{10}O$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			13	12 1		
3	B	1	Total	C O	0	0
			13	12 1		

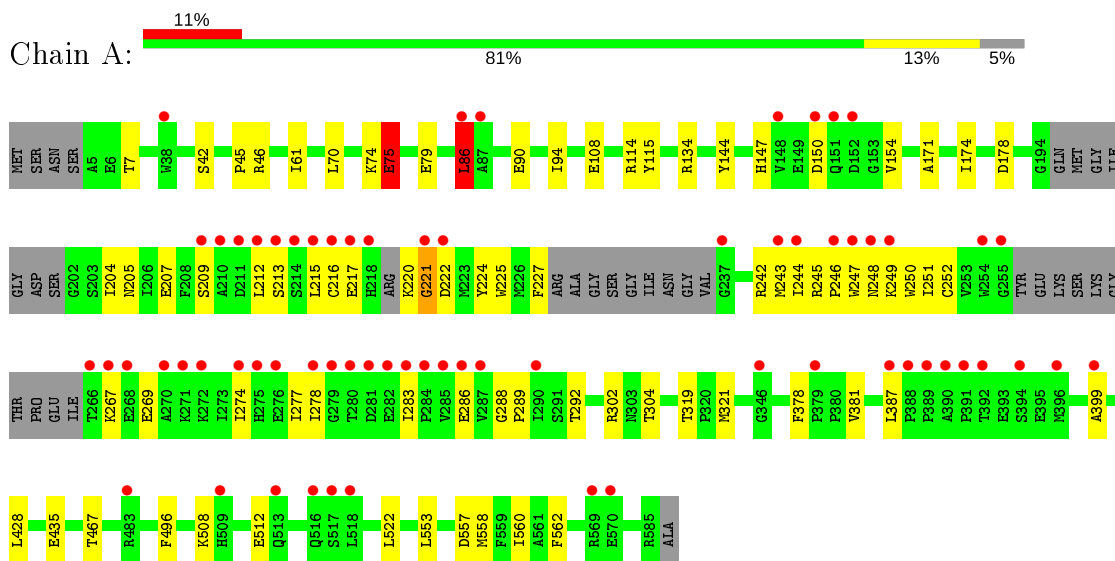
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	423	Total	O	0	0
			423	423		
4	B	417	Total	O	0	0
			417	417		

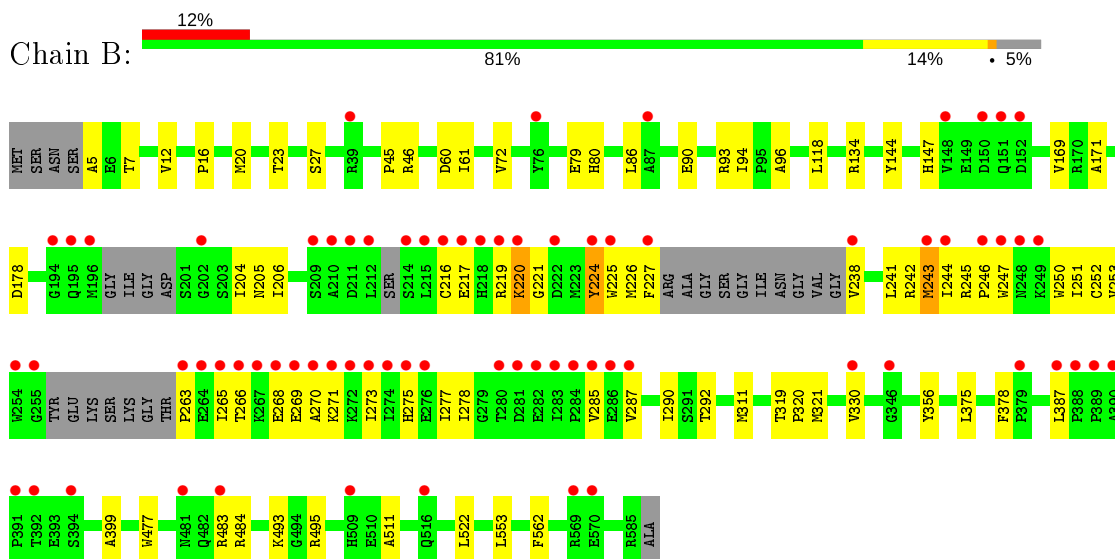
3 Residue-property plots [i](#)

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: 2-hydroxybiphenyl-3-monooxygenase



- Molecule 1: 2-hydroxybiphenyl-3-monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.47Å 130.68Å 78.66Å 90.00° 98.61° 90.00°	Depositor
Resolution (Å)	36.30 – 2.30 36.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.30-2.30) 99.5 (36.30-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.08 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.229 , 0.255 0.222 , 0.247	Depositor DCC
R_{free} test set	5149 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtrriage
Anisotropy	0.650	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9534	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8199e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CH9, 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	0.46	2/4350 (0.0%)	0.64	6/5894 (0.1%)
1	B	0.43	0/4396	0.61	4/5955 (0.1%)
All	All	0.45	2/8746 (0.0%)	0.62	10/11849 (0.1%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	GLU	C-N	-10.96	1.08	1.34
1	A	74	LYS	C-N	-8.84	1.13	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	75	GLU	O-C-N	-12.63	102.49	122.70
1	A	221	GLY	N-CA-C	-8.36	92.20	113.10
1	B	243	MET	O-C-N	8.05	135.58	122.70
1	B	118	LEU	CB-CG-CD1	-7.35	98.51	111.00
1	B	243	MET	CA-C-N	-6.39	103.13	117.20
1	A	75	GLU	CA-C-N	6.04	130.49	117.20
1	B	263	PRO	N-CA-CB	5.86	110.34	103.30
1	A	86	LEU	CA-CB-CG	5.78	128.60	115.30
1	A	217	GLU	C-N-CA	5.62	135.76	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ASP	N-CA-CB	-5.24	101.17	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	GLU	Mainchain

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	4258	0	4205	58	0
1	B	4304	0	4254	75	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	13	0	10	4	0
3	B	13	0	10	2	0
4	A	423	0	0	1	0
4	B	417	0	0	0	1
All	All	9534	0	8541	135	1

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 8.

All (135) 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:B:243:MET:HA	1:B:250:TRP:CZ3	2.08	0.88
1:A:154:VAL:HG21	1:A:174:ILE:HG13	1.64	0.78
1:B:243:MET:HA	1:B:250:TRP:HZ3	1.50	0.76
1:B:219:ARG:HG3	1:B:220:LYS:H	1.50	0.75
1:B:86:LEU:HD23	1:B:278:ILE:HG23	1.68	0.74
1:B:86:LEU:HD13	1:B:241:LEU:HD23	1.70	0.73
1:B:60:ASP:O	1:B:493:LYS:NZ	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ARG:HG3	1:B:220:LYS:N	2.04	0.70
1:B:72:VAL:HG21	1:B:243:MET:HE2	1.74	0.70
1:B:90:GLU:OE2	1:B:93:ARG:NH2	2.23	0.70
1:A:94:ILE:HD11	1:A:428:LEU:HD12	1.74	0.69
1:A:79:GLU:HB2	1:A:221:GLY:N	2.07	0.69
1:A:205:ASN:HB3	1:A:251:ILE:HD11	1.75	0.69
1:B:243:MET:CA	1:B:250:TRP:HZ3	2.06	0.68
1:B:219:ARG:CG	1:B:220:LYS:H	2.09	0.66
1:A:278:ILE:HD11	1:A:283:ILE:HD12	1.78	0.66
1:A:79:GLU:HB2	1:A:220:LYS:C	2.16	0.65
1:A:86:LEU:HD21	1:A:212:LEU:HD13	1.77	0.65
3:A:602:CH9:OAA	3:A:602:CH9:HAH	1.96	0.65
1:B:219:ARG:NH2	1:B:224:TYR:CD1	2.66	0.64
1:A:86:LEU:CD1	1:A:215:LEU:HB3	2.27	0.63
1:B:227:PHE:CD1	1:B:238:VAL:HG12	2.32	0.63
1:A:207:GLU:O	1:A:288:GLY:N	2.32	0.63
1:B:144:TYR:OH	1:B:147:HIS:HD2	1.81	0.63
1:A:212:LEU:HD23	1:A:283:ILE:HD13	1.82	0.62
1:A:94:ILE:HD11	1:A:428:LEU:CD1	2.30	0.61
1:A:144:TYR:OH	1:A:147:HIS:HD2	1.82	0.61
1:B:219:ARG:NE	1:B:224:TYR:CE1	2.68	0.61
1:B:219:ARG:O	1:B:220:LYS:HB2	2.00	0.60
1:B:79:GLU:O	1:B:221:GLY:HA3	2.01	0.60
1:B:80:HIS:CD2	1:B:94:ILE:HD11	2.36	0.60
1:A:225:TRP:CZ3	1:A:378:PHE:CE1	2.89	0.60
1:B:216:CYS:HG	1:B:224:TYR:HE1	1.50	0.59
1:B:220:LYS:HD3	1:B:247:TRP:HZ2	1.68	0.59
1:B:321:MET:SD	3:B:602:CH9:HAJ	2.43	0.59
1:B:45:PRO:HB2	1:B:242:ARG:NH2	2.18	0.58
1:B:319:THR:HG21	1:B:375:LEU:HD11	1.86	0.58
1:B:219:ARG:CG	1:B:220:LYS:N	2.67	0.58
1:B:219:ARG:HE	1:B:224:TYR:HE1	1.52	0.57
1:B:204:ILE:HD11	1:B:290:ILE:HG22	1.85	0.57
1:B:268:GLU:O	1:B:271:LYS:HB3	2.04	0.57
1:B:219:ARG:NH2	1:B:224:TYR:HD1	2.01	0.56
1:A:274:ILE:O	1:A:278:ILE:HG22	2.06	0.56
1:A:86:LEU:HD12	1:A:215:LEU:HD23	1.87	0.56
1:A:46:ARG:O	1:A:242:ARG:NH2	2.39	0.56
1:A:61:ILE:O	1:A:134:ARG:NH2	2.40	0.55
1:A:248:ASN:N	1:A:248:ASN:OD1	2.39	0.55
1:A:70:LEU:O	1:A:245:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:CYS:SG	1:A:277:ILE:HD13	2.46	0.55
1:B:219:ARG:NE	1:B:224:TYR:HE1	2.05	0.54
1:B:80:HIS:HE1	1:B:225:TRP:CD1	2.26	0.54
1:B:243:MET:CA	1:B:250:TRP:CZ3	2.84	0.53
1:B:553:LEU:HB3	1:B:562:PHE:HB3	1.91	0.53
1:B:72:VAL:HG21	1:B:243:MET:CE	2.39	0.53
1:A:204:ILE:HG12	1:A:292:THR:HG22	1.90	0.52
1:B:511:ALA:HB1	1:B:522:LEU:HD22	1.91	0.52
1:B:244:ILE:O	1:B:245:ARG:HD3	2.10	0.52
1:A:243:MET:HA	1:A:250:TRP:CZ3	2.45	0.52
1:A:553:LEU:HB3	1:A:562:PHE:HB3	1.92	0.52
1:B:46:ARG:O	1:B:242:ARG:NH2	2.43	0.52
1:B:27:SER:OG	1:B:134:ARG:HD3	2.10	0.51
1:A:220:LYS:HA	1:A:247:TRP:CH2	2.45	0.51
1:A:207:GLU:CD	1:A:289:PRO:HG2	2.30	0.51
1:B:227:PHE:HD1	1:B:238:VAL:HG12	1.76	0.51
1:B:220:LYS:HD3	1:B:247:TRP:CZ2	2.46	0.50
1:B:61:ILE:O	1:B:134:ARG:NH2	2.45	0.50
1:A:321:MET:SD	3:A:602:CH9:HAJ	2.52	0.50
1:B:387:LEU:HD21	1:B:399:ALA:HB2	1.93	0.49
1:B:217:GLU:O	1:B:220:LYS:HE2	2.13	0.49
1:B:252:CYS:SG	1:B:277:ILE:HD13	2.53	0.48
1:A:225:TRP:HZ3	1:A:378:PHE:CE1	2.30	0.48
1:A:212:LEU:CD2	1:A:283:ILE:HD13	2.42	0.48
1:B:269:GLU:O	1:B:273:ILE:N	2.41	0.48
1:B:219:ARG:CZ	1:B:224:TYR:CE1	2.96	0.48
1:A:108:GLU:HG3	1:A:114:ARG:NH2	2.29	0.47
1:B:226:MET:HG3	1:B:277:ILE:HG23	1.96	0.47
1:B:7:THR:O	1:B:171:ALA:HA	2.13	0.47
1:A:86:LEU:HD12	1:A:215:LEU:HB3	1.95	0.47
1:A:244:ILE:O	1:A:245:ARG:HD3	2.14	0.47
1:B:205:ASN:HB3	1:B:251:ILE:HD11	1.97	0.47
1:A:207:GLU:OE2	1:A:289:PRO:HG2	2.15	0.47
1:A:508:LYS:O	1:A:512:GLU:HG3	2.15	0.47
1:A:79:GLU:N	1:A:221:GLY:HA2	2.30	0.46
1:A:496:PHE:HB2	1:A:522:LEU:HD23	1.97	0.46
3:A:602:CH9:OAA	3:A:602:CH9:CAH	2.63	0.46
1:B:219:ARG:O	1:B:220:LYS:CB	2.63	0.46
1:A:227:PHE:CZ	1:A:381:VAL:HG11	2.50	0.46
1:A:243:MET:SD	1:A:243:MET:C	2.94	0.46
1:B:247:TRP:HE3	1:B:250:TRP:CH2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LYS:CD	1:B:247:TRP:HZ2	2.29	0.45
1:A:207:GLU:O	1:A:288:GLY:CA	2.65	0.45
1:B:206:ILE:HD13	1:B:270:ALA:HB1	1.99	0.45
1:A:302:ARG:NH1	1:A:304:THR:O	2.50	0.45
1:B:220:LYS:HA	1:B:247:TRP:CZ2	2.52	0.45
1:B:271:LYS:HB2	1:B:287:VAL:HG21	1.99	0.45
1:A:144:TYR:OH	1:A:147:HIS:CD2	2.67	0.44
1:B:243:MET:HA	1:B:250:TRP:CE3	2.52	0.44
1:B:271:LYS:HZ1	1:B:285:VAL:HG13	1.82	0.44
1:B:271:LYS:HZ2	1:B:275:HIS:CE1	2.35	0.44
1:B:86:LEU:HB3	1:B:278:ILE:O	2.17	0.44
1:A:42:SER:OG	1:A:46:ARG:NH1	2.50	0.44
1:A:7:THR:O	1:A:171:ALA:HA	2.17	0.44
1:B:204:ILE:HD13	1:B:292:THR:HG22	1.99	0.44
1:A:86:LEU:CD1	1:A:215:LEU:CB	2.94	0.44
1:A:213:SER:HA	1:A:216:CYS:SG	2.58	0.44
1:B:12:VAL:HG12	1:B:178:ASP:HB3	2.00	0.44
1:A:79:GLU:O	1:A:221:GLY:HA3	2.18	0.43
1:A:249:LYS:NZ	4:A:726:HOH:O	2.48	0.43
1:B:225:TRP:CZ3	1:B:378:PHE:CE1	3.05	0.43
1:A:246:PRO:HA	1:A:247:TRP:HA	1.51	0.43
1:B:5:ALA:HB3	1:B:169:VAL:HG22	1.98	0.43
1:B:246:PRO:HA	1:B:247:TRP:HA	1.54	0.43
1:B:277:ILE:HG22	1:B:277:ILE:O	2.18	0.43
1:A:321:MET:SD	3:A:602:CH9:HAI	2.59	0.42
1:A:387:LEU:HD21	1:A:399:ALA:HB2	2.01	0.42
1:A:557:ASP:O	1:A:558:MET:HB2	2.19	0.42
1:B:20:MET:HG2	1:B:330:VAL:HG13	2.01	0.42
1:A:209:SER:HB2	1:A:286:GLU:HB3	2.01	0.42
1:A:467:THR:HA	1:A:560:ILE:HD12	2.02	0.42
1:B:477:TRP:HB3	1:B:484:ARG:HG2	2.02	0.42
1:B:320:PRO:HG2	3:B:602:CH9:CAH	2.49	0.42
1:B:205:ASN:OD1	1:B:253:VAL:HG13	2.20	0.42
1:B:23:THR:HG23	1:B:134:ARG:HD2	2.02	0.41
1:A:154:VAL:HG21	1:A:174:ILE:CG1	2.44	0.41
1:A:45:PRO:HB2	1:A:242:ARG:NH2	2.34	0.41
1:B:245:ARG:O	1:B:247:TRP:HA	2.21	0.41
1:B:86:LEU:HB2	1:B:278:ILE:HA	2.03	0.41
1:B:80:HIS:CE1	1:B:225:TRP:CD1	3.06	0.41
1:B:311:MET:HB3	1:B:356:TYR:OH	2.21	0.41
1:A:115:TYR:OH	1:A:435:GLU:OE2	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:CD1	1:A:428:LEU:HD12	2.46	0.41
1:B:238:VAL:O	1:B:238:VAL:HG23	2.21	0.41
1:A:267:LYS:H	1:A:269:GLU:CG	2.34	0.40
1:B:16:PRO:HD2	2:B:601:FAD:O2P	2.22	0.40
1:A:178:ASP:N	1:A:178:ASP:OD1	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:749:HOH:O	4:B:964:HOH:O[2_655]	2.15	0.05

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	544/586 (93%)	525 (96%)	18 (3%)	1 (0%)	47 58
1	B	549/586 (94%)	523 (95%)	22 (4%)	4 (1%)	22 26
All	All	1093/1172 (93%)	1048 (96%)	40 (4%)	5 (0%)	29 35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	220	LYS
1	B	266	THR
1	B	96	ALA
1	A	75	GLU
1	B	265	ILE

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	443/467 (95%)	438 (99%)	5 (1%)	73	86
1	B	448/467 (96%)	445 (99%)	3 (1%)	84	92
All	All	891/934 (95%)	883 (99%)	8 (1%)	78	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	90	GLU
1	A	150	ASP
1	A	224	TYR
1	A	319	THR
1	B	224	TYR
1	B	483	ARG
1	B	495	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	509	HIS
1	B	80	HIS
1	B	147	HIS

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](#)

4 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
3	CH9	B	602	-	14,14,14	3.12	7 (50%)	18,18,18	0.53	0
3	CH9	A	602	-	14,14,14	3.06	7 (50%)	18,18,18	0.99	1 (5%)
2	FAD	B	601	-	51,58,58	2.79	15 (29%)	60,89,89	2.00	16 (26%)
2	FAD	A	601	-	51,58,58	2.73	17 (33%)	60,89,89	2.06	16 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CH9	B	602	-	-	1/4/4/4	0/2/2/2
3	CH9	A	602	-	-	4/4/4/4	0/2/2/2
2	FAD	B	601	-	1/1/9/9	13/30/50/50	0/6/6/6
2	FAD	A	601	-	1/1/9/9	11/30/50/50	0/6/6/6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C4X-C10	12.61	1.51	1.38
2	A	601	FAD	C4X-C10	11.63	1.50	1.38
2	B	601	FAD	C5X-N5	8.10	1.48	1.35
2	A	601	FAD	C5X-N5	7.97	1.48	1.35
3	B	602	CH9	CAC-CAH	5.06	1.49	1.38
3	A	602	CH9	CAE-CAG	4.96	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	CH9	CAE-CAG	4.95	1.49	1.38
3	B	602	CH9	CAF-CAJ	4.89	1.49	1.38
3	A	602	CH9	CAC-CAH	4.88	1.49	1.38
3	A	602	CH9	CAF-CAJ	4.86	1.49	1.38
2	B	601	FAD	C2'-C3'	4.81	1.62	1.53
3	B	602	CH9	CAI-CAL	4.73	1.49	1.39
3	A	602	CH9	CAI-CAL	4.57	1.49	1.39
2	A	601	FAD	C1'-N10	-4.56	1.43	1.48
3	B	602	CH9	CAD-CAB	4.33	1.49	1.38
3	A	602	CH9	CAD-CAB	4.19	1.49	1.38
2	A	601	FAD	C2'-C3'	4.17	1.61	1.53
2	A	601	FAD	C2B-C1B	-4.03	1.47	1.53
2	B	601	FAD	C2-N1	4.03	1.46	1.38
2	B	601	FAD	C2B-C1B	-3.96	1.47	1.53
2	A	601	FAD	C4-N3	3.93	1.39	1.33
2	A	601	FAD	C2-N1	3.83	1.45	1.38
2	B	601	FAD	C4-N3	3.59	1.39	1.33
2	B	601	FAD	C4-C4X	3.33	1.47	1.41
3	B	602	CH9	CAM-CAK	3.28	1.50	1.40
2	A	601	FAD	C4-C4X	3.14	1.46	1.41
2	B	601	FAD	C9A-N10	3.10	1.42	1.38
3	A	602	CH9	CAM-CAK	2.92	1.49	1.40
2	B	601	FAD	C1'-N10	-2.92	1.45	1.48
2	B	601	FAD	C2A-N3A	2.83	1.36	1.32
2	A	601	FAD	C2A-N3A	2.83	1.36	1.32
2	A	601	FAD	C6A-N6A	2.62	1.43	1.34
2	B	601	FAD	C6A-N6A	2.58	1.43	1.34
2	A	601	FAD	O2'-C2'	2.57	1.48	1.43
2	A	601	FAD	O2B-C2B	-2.50	1.37	1.43
2	A	601	FAD	C9A-N10	2.48	1.41	1.38
2	B	601	FAD	O2'-C2'	2.46	1.48	1.43
2	B	601	FAD	O2B-C2B	-2.36	1.37	1.43
3	A	602	CH9	CAJ-CAM	-2.36	1.36	1.40
2	B	601	FAD	O3B-C3B	-2.32	1.37	1.43
2	B	601	FAD	O3'-C3'	-2.27	1.37	1.43
2	A	601	FAD	O3B-C3B	-2.19	1.37	1.43
3	B	602	CH9	CAJ-CAM	-2.18	1.36	1.40
2	A	601	FAD	O4B-C4B	-2.15	1.40	1.45
2	A	601	FAD	C2-N3	2.12	1.42	1.38
2	A	601	FAD	O3'-C3'	-2.08	1.38	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4-N3-C2	6.83	120.91	115.14
2	B	601	FAD	C4-N3-C2	6.76	120.85	115.14
2	B	601	FAD	N3A-C2A-N1A	-6.11	119.14	128.68
2	A	601	FAD	N3A-C2A-N1A	-5.82	119.58	128.68
2	A	601	FAD	O2P-P-O5'	-5.49	82.26	107.75
2	B	601	FAD	O2P-P-O5'	-5.42	82.57	107.75
2	B	601	FAD	O5'-P-O1P	-5.21	88.71	109.07
2	A	601	FAD	O5'-P-O1P	-4.77	90.44	109.07
2	A	601	FAD	C4-C4X-C10	-3.76	117.46	119.95
2	A	601	FAD	O2'-C2'-C3'	3.31	117.16	109.10
2	A	601	FAD	C5'-C4'-C3'	3.31	118.60	112.20
2	A	601	FAD	C4X-N5-C5X	3.11	119.88	116.77
3	A	602	CH9	CAL-CAM-CAK	-3.07	119.67	122.36
2	A	601	FAD	C4-C4X-N5	3.05	122.09	118.60
2	B	601	FAD	O2'-C2'-C3'	2.93	116.21	109.10
2	B	601	FAD	C4X-C4-N3	-2.86	119.53	123.43
2	B	601	FAD	C4'-C3'-C2'	2.83	119.25	113.36
2	A	601	FAD	O3'-C3'-C4'	2.69	115.30	108.81
2	A	601	FAD	C4X-C4-N3	-2.68	119.77	123.43
2	B	601	FAD	C4-C4X-C10	-2.66	118.19	119.95
2	A	601	FAD	C4X-C10-N10	-2.64	117.59	120.30
2	B	601	FAD	C1'-C2'-C3'	2.60	117.07	109.79
2	B	601	FAD	C4X-N5-C5X	2.42	119.19	116.77
2	B	601	FAD	C5'-C4'-C3'	2.41	116.85	112.20
2	A	601	FAD	C2A-N1A-C6A	2.32	122.73	118.75
2	B	601	FAD	C1B-N9A-C4A	-2.30	122.60	126.64
2	A	601	FAD	C1B-N9A-C4A	-2.27	122.65	126.64
2	A	601	FAD	C4'-C3'-C2'	2.27	118.08	113.36
2	B	601	FAD	C2A-N1A-C6A	2.19	122.49	118.75
2	B	601	FAD	C4X-C10-N10	-2.18	118.06	120.30
2	A	601	FAD	C4A-C5A-N7A	-2.18	107.13	109.40
2	B	601	FAD	C4A-C5A-N7A	-2.10	107.21	109.40
2	B	601	FAD	C4-C4X-N5	2.07	120.97	118.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	601	FAD	C3'
2	A	601	FAD	C3'

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C1'-C2'-C3'-O3'
2	B	601	FAD	C1'-C2'-C3'-C4'
2	B	601	FAD	O2'-C2'-C3'-O3'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	B	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C1'-C2'-C3'-O3'
2	A	601	FAD	C1'-C2'-C3'-C4'
2	A	601	FAD	O2'-C2'-C3'-O3'
2	A	601	FAD	O2'-C2'-C3'-C4'
2	A	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-C5'
3	A	602	CH9	CAH-CAL-CAM-CAJ
3	A	602	CH9	CAI-CAL-CAM-CAJ
3	A	602	CH9	CAH-CAL-CAM-CAK
2	B	601	FAD	P-O3P-PA-O5B
2	A	601	FAD	P-O3P-PA-O5B
3	A	602	CH9	CAI-CAL-CAM-CAK
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
3	B	602	CH9	CAI-CAL-CAM-CAJ
2	B	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	PA-O3P-P-O2P
2	B	601	FAD	C5'-O5'-P-O1P
2	A	601	FAD	C5'-O5'-P-O1P

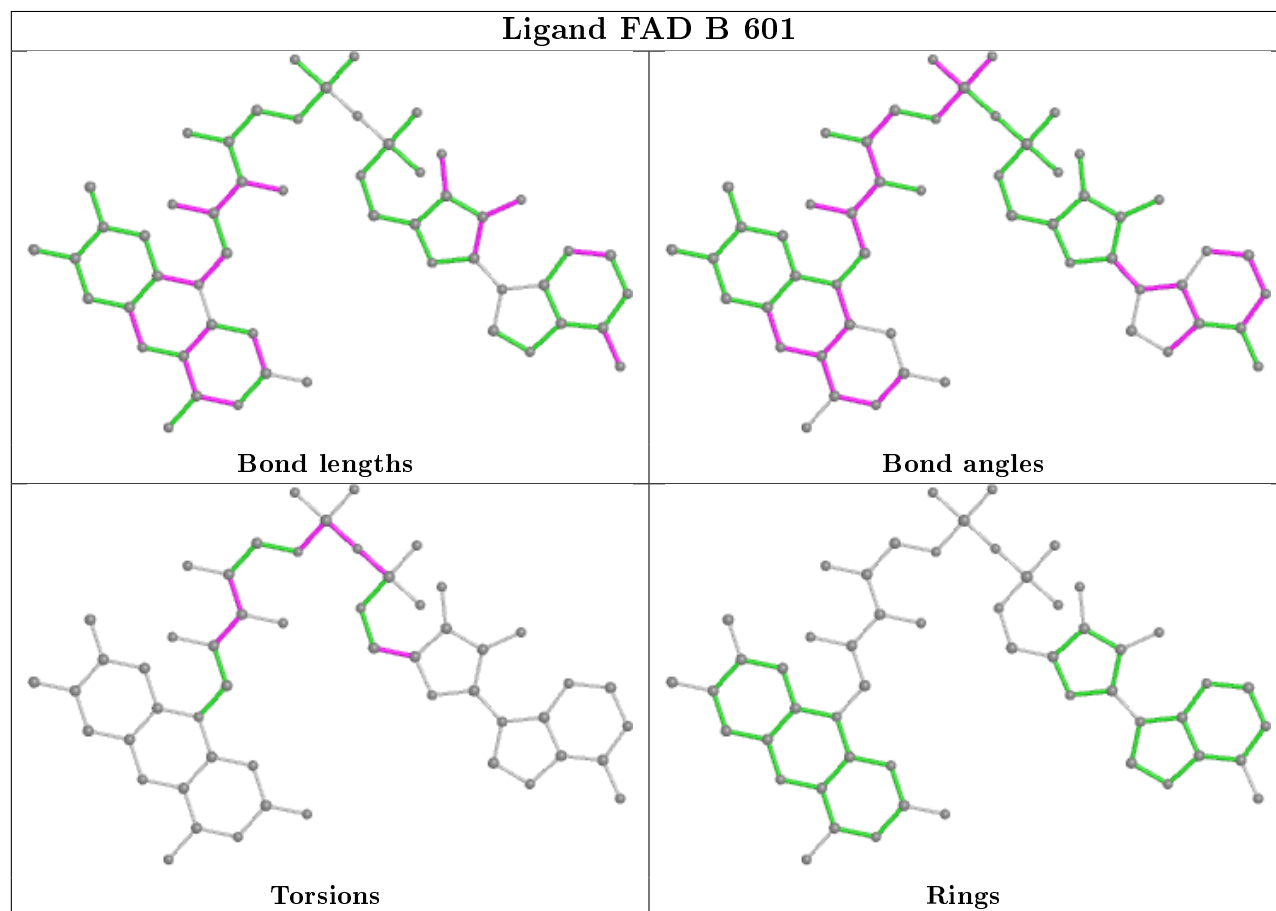
There are no ring outliers.

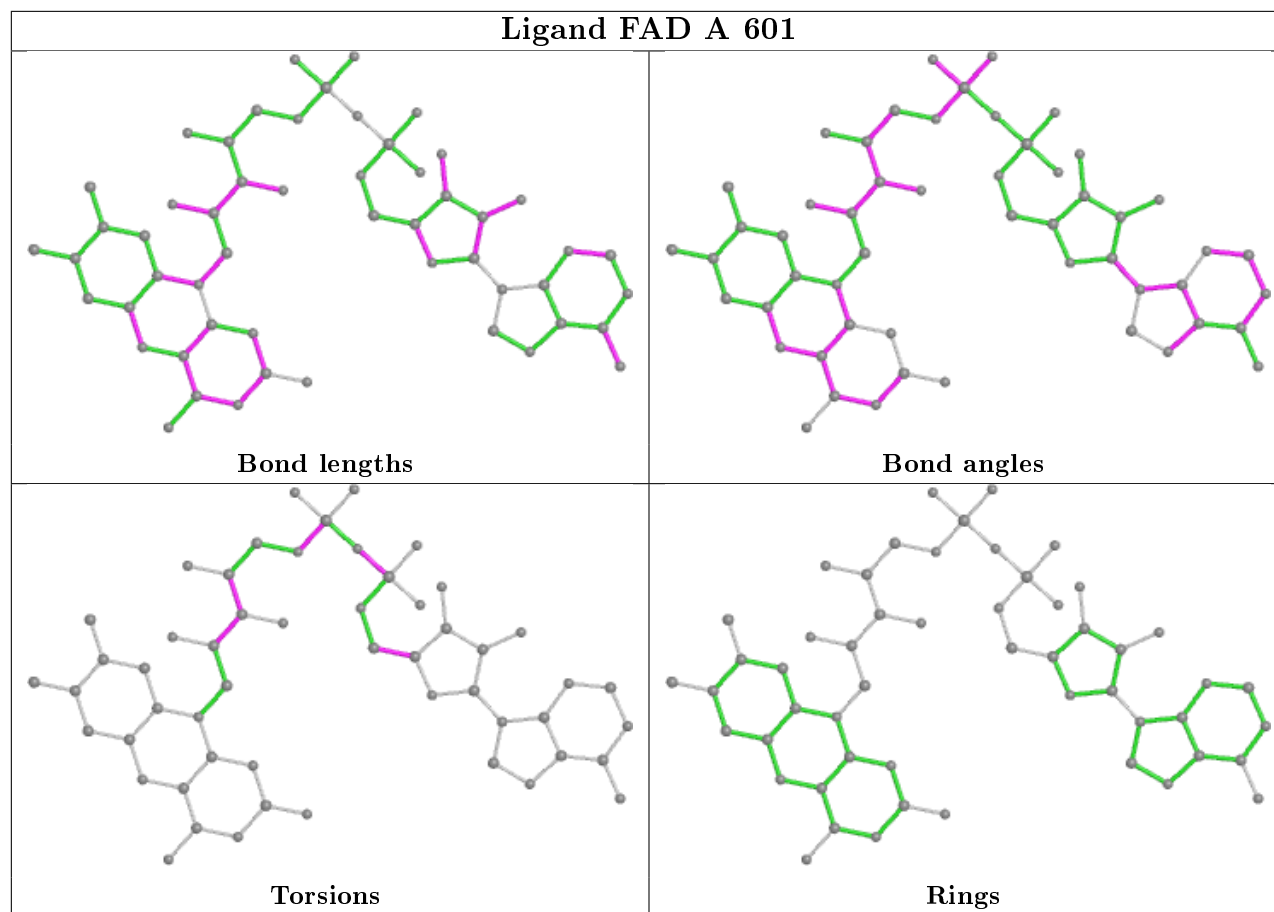
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	CH9	2	0
3	A	602	CH9	4	0
2	B	601	FAD	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	74:LYS	C	75:GLU	N	1.13
1	A	75:GLU	C	76:TYR	N	1.08

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	554/586 (94%)	0.59	67 (12%) 4 6	12, 25, 78, 136	0
1	B	559/586 (95%)	0.55	73 (13%) 3 4	10, 25, 80, 142	0
All	All	1113/1172 (94%)	0.57	140 (12%) 3 5	10, 25, 80, 142	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	PRO	13.5
1	B	282	GLU	12.2
1	A	282	GLU	9.1
1	A	213	SER	8.6
1	A	212	LEU	8.4
1	B	265	ILE	7.9
1	A	210	ALA	7.8
1	B	216	CYS	7.6
1	B	249	LYS	7.4
1	A	285	VAL	7.4
1	A	218	HIS	6.7
1	A	151	GLN	6.6
1	A	270	ALA	6.5
1	B	243	MET	6.4
1	B	271	LYS	6.1
1	A	211	ASP	5.9
1	A	390	ALA	5.8
1	B	285	VAL	5.5
1	A	246	PRO	5.3
1	A	388	PRO	5.3
1	B	210	ALA	5.3
1	A	247	TRP	5.2
1	B	151	GLN	5.0
1	B	219	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	281	ASP	5.0
1	B	217	GLU	5.0
1	A	394	SER	5.0
1	B	270	ALA	5.0
1	B	248	ASN	4.9
1	B	275	HIS	4.9
1	B	272	LYS	4.8
1	B	247	TRP	4.8
1	A	209	SER	4.7
1	A	389	PRO	4.7
1	B	268	GLU	4.7
1	A	276	GLU	4.7
1	A	271	LYS	4.7
1	A	391	PRO	4.6
1	A	272	LYS	4.6
1	A	267	LYS	4.5
1	B	390	ALA	4.5
1	A	283	ILE	4.5
1	A	237	GLY	4.4
1	B	195	GLN	4.4
1	B	283	ILE	4.4
1	A	275	HIS	4.4
1	B	388	PRO	4.4
1	A	274	ILE	4.3
1	B	218	HIS	4.3
1	A	280	THR	4.3
1	B	264	GLU	4.3
1	A	249	LYS	4.3
1	A	392	THR	4.3
1	B	212	LEU	4.2
1	A	248	ASN	4.2
1	A	287	VAL	4.1
1	A	243	MET	4.1
1	B	209	SER	4.1
1	A	284	PRO	4.0
1	A	221	GLY	4.0
1	A	516	GLN	4.0
1	A	569	ARG	3.9
1	B	266	THR	3.9
1	B	394	SER	3.8
1	B	391	PRO	3.8
1	B	202	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	392	THR	3.7
1	B	211	ASP	3.7
1	B	280	THR	3.6
1	B	220	LYS	3.6
1	A	387	LEU	3.5
1	A	268	GLU	3.5
1	A	215	LEU	3.5
1	A	286	GLU	3.4
1	B	269	GLU	3.4
1	B	483	ARG	3.4
1	B	215	LEU	3.4
1	A	483	ARG	3.3
1	B	569	ARG	3.3
1	B	246	PRO	3.3
1	B	196	MET	3.3
1	A	38	TRP	3.3
1	B	274	ILE	3.2
1	A	379	PRO	3.2
1	A	216	CYS	3.2
1	A	217	GLU	3.1
1	B	570	GLU	3.1
1	B	387	LEU	3.1
1	A	509	HIS	3.1
1	A	87	ALA	3.0
1	A	86	LEU	2.9
1	B	286	GLU	2.9
1	A	222	ASP	2.9
1	A	290	ILE	2.9
1	B	150	ASP	2.9
1	B	281	ASP	2.8
1	B	284	PRO	2.8
1	A	396	MET	2.8
1	A	148	VAL	2.8
1	A	150	ASP	2.8
1	A	399	ALA	2.7
1	B	238	VAL	2.7
1	B	267	LYS	2.7
1	A	279	GLY	2.7
1	B	330	VAL	2.7
1	B	194	GLY	2.7
1	B	87	ALA	2.6
1	A	266	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	278	ILE	2.6
1	B	276	GLU	2.6
1	B	222	ASP	2.6
1	B	379	PRO	2.6
1	B	225	TRP	2.5
1	B	509	HIS	2.5
1	B	39	ARG	2.5
1	A	244	ILE	2.5
1	B	244	ILE	2.5
1	B	346	GLY	2.5
1	A	517	SER	2.5
1	B	287	VAL	2.5
1	A	513	GLN	2.5
1	B	227	PHE	2.4
1	B	481	ASN	2.4
1	B	224	TYR	2.4
1	A	254	TRP	2.4
1	A	255	GLY	2.3
1	A	346	GLY	2.3
1	B	152	ASP	2.3
1	B	148	VAL	2.3
1	B	76	TYR	2.2
1	A	570	GLU	2.2
1	B	516	GLN	2.2
1	A	518	LEU	2.2
1	B	214	SER	2.2
1	A	152	ASP	2.2
1	B	389	PRO	2.2
1	B	255	GLY	2.2
1	B	273	ILE	2.2
1	A	214	SER	2.2
1	B	254	TRP	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](#)

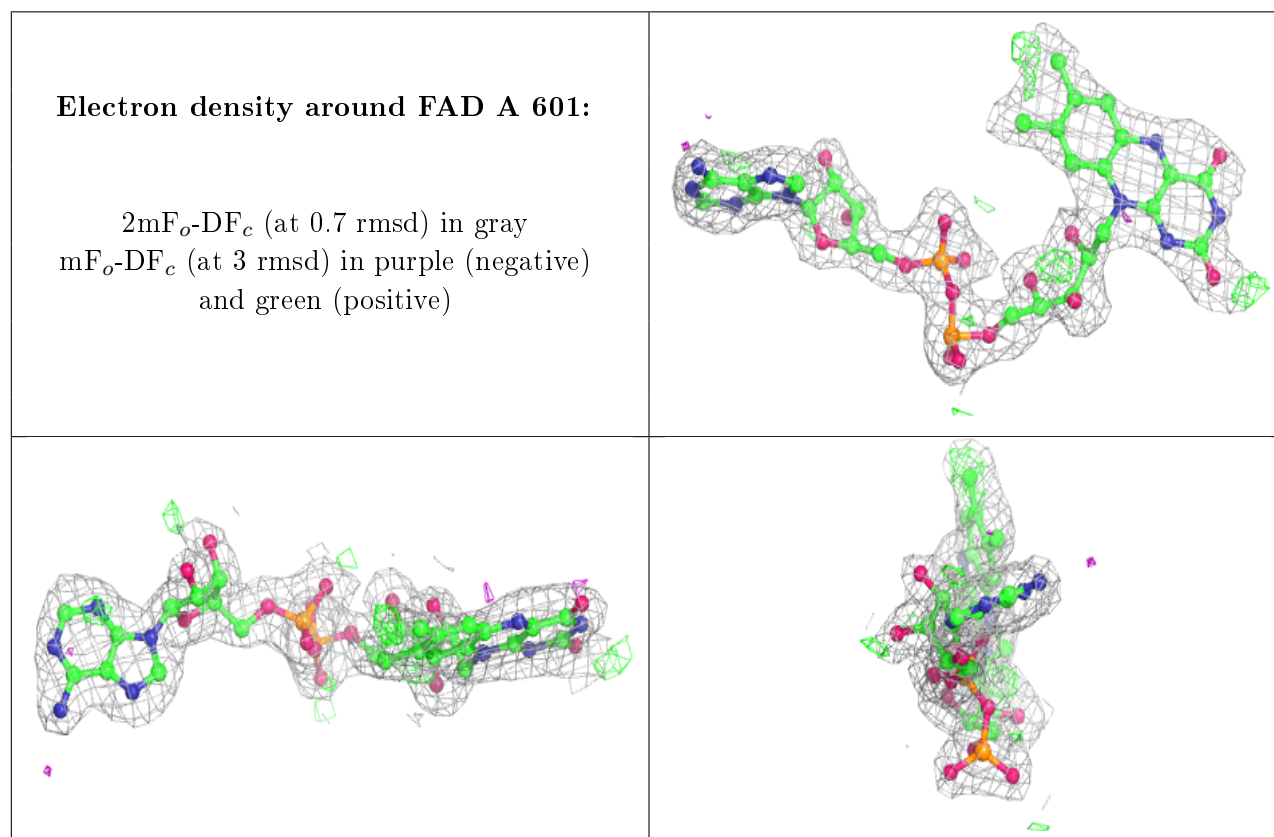
There are no carbohydrates in this entry.

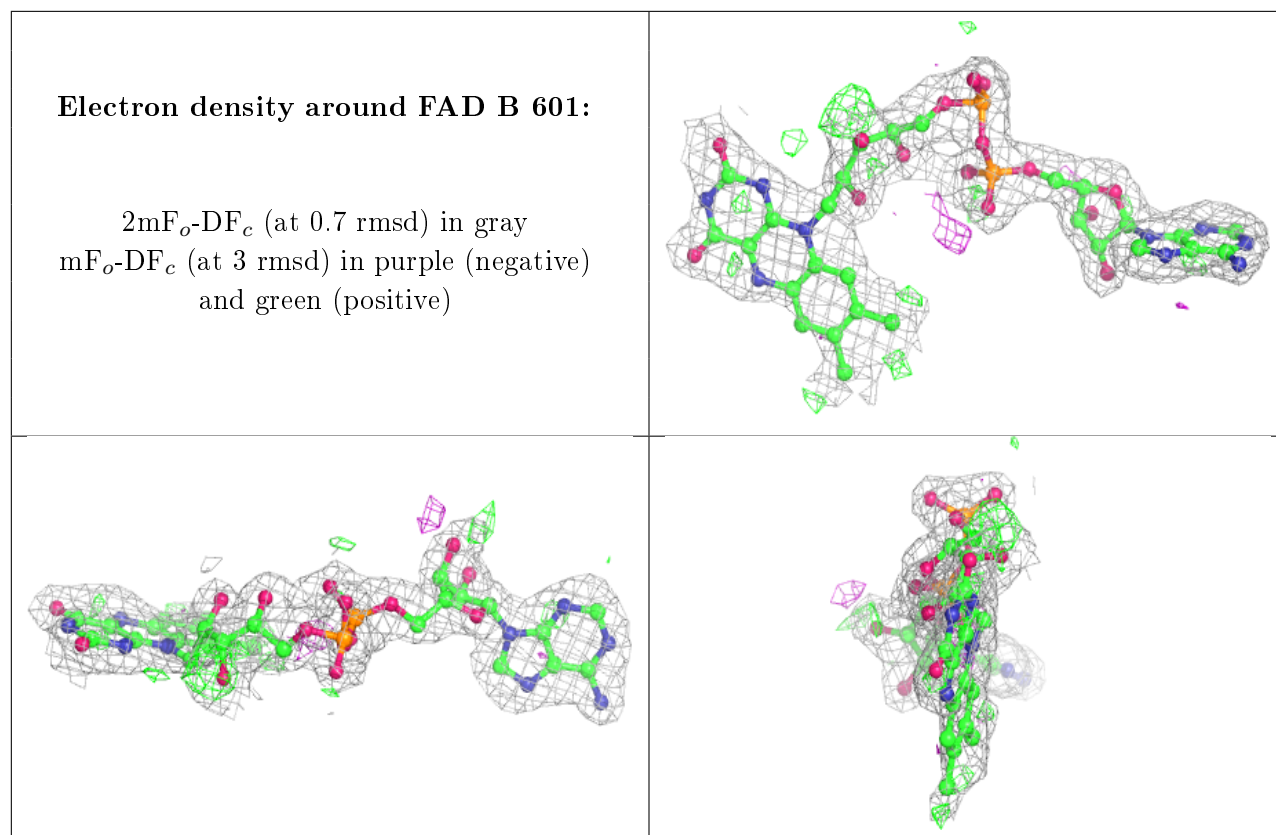
6.4 Ligands [\(i\)](#)

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	CH9	B	602	13/13	0.76	0.26	59,63,64,65	0
3	CH9	A	602	13/13	0.80	0.33	58,60,64,64	0
2	FAD	A	601	53/53	0.93	0.14	20,31,41,46	0
2	FAD	B	601	53/53	0.94	0.13	17,27,43,47	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.