



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:37 PM UTC

PDB ID : 5BRT / pdb_00005brt
Title : Crystal Structure of 2-hydroxybiphenyl 3-monooxygenase from *Pseudomonas azelaica* with 2-hydroxybiphenyl in the active site
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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 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

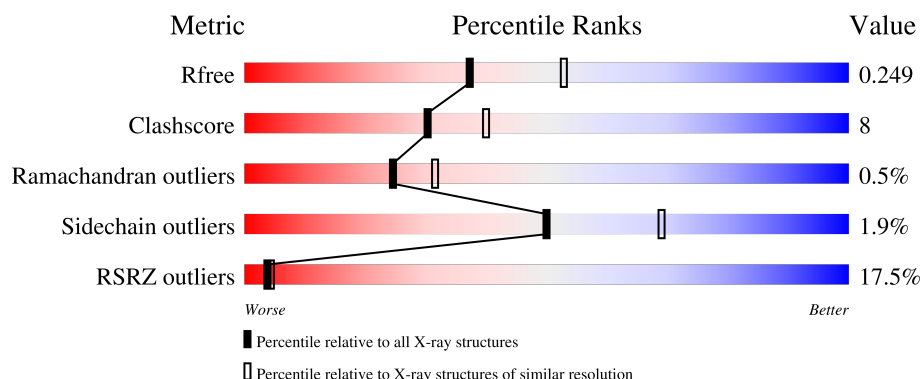
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



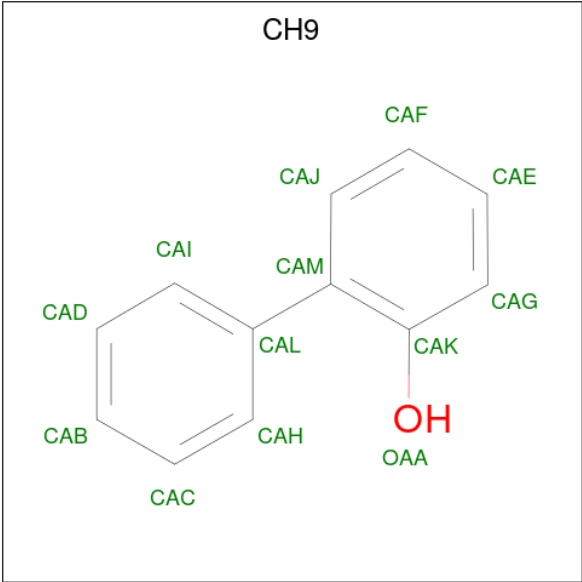
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 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	586	17% 79% 14% • 5%
1	B	586	17% 80% 14% • 5%

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	-	-	-



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		

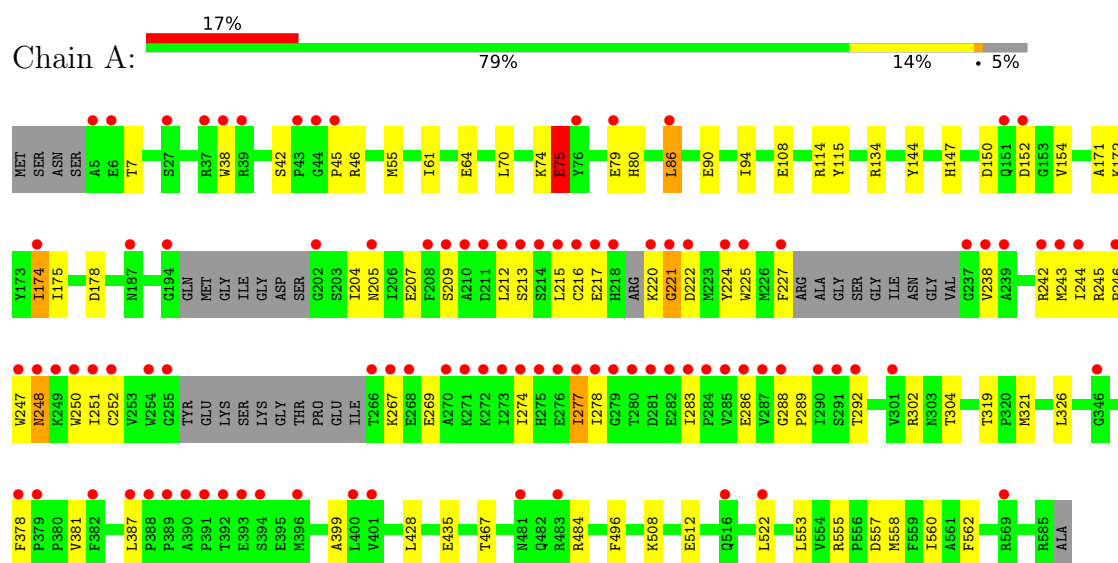
- Molecule 4 is water.

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

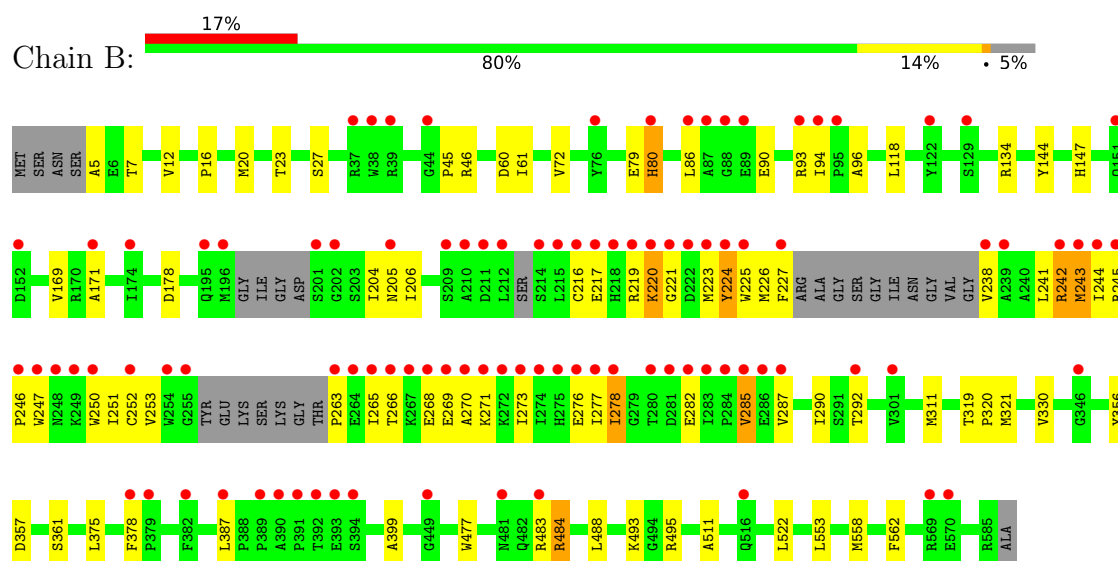
3 Residue-property plots

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: 2-hydroxybiphenyl-3-monooxygenase



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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 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.30-2.30) 99.6 (36.30-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.08 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.229 , 0.255 0.224 , 0.249	Depositor DCC
R_{free} test set	5152 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9534	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage'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.*

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: 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	0.62	3/4350 (0.1%)	0.91	10/5894 (0.2%)
1	B	0.56	3/4396 (0.1%)	0.87	7/5955 (0.1%)
All	All	0.59	6/8746 (0.1%)	0.89	17/11849 (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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	GLU	C-N	-18.02	1.08	1.33
1	A	74	LYS	C-N	-14.26	1.13	1.33
1	B	243	MET	C-N	11.67	1.45	1.33
1	A	217	GLU	C-N	-7.45	1.23	1.33
1	B	242	ARG	C-N	6.48	1.42	1.33
1	B	118	LEU	CG-CD1	-5.74	1.33	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	GLU	O-C-N	-15.11	102.49	122.59
1	A	221	GLY	N-CA-C	-14.94	92.20	112.82
1	B	243	MET	CA-C-N	-11.08	109.45	122.63
1	B	243	MET	C-N-CA	-11.08	109.45	122.63
1	B	243	MET	O-C-N	10.85	135.58	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	HIS	N-CA-C	8.32	121.82	109.59
1	A	217	GLU	CA-C-N	7.81	135.76	121.70
1	A	217	GLU	C-N-CA	7.81	135.76	121.70
1	B	80	HIS	CA-C-N	-7.71	112.42	123.06
1	B	80	HIS	C-N-CA	-7.71	112.42	123.06
1	A	152	ASP	N-CA-C	-7.33	104.86	114.31
1	B	263	PRO	N-CA-CB	6.67	110.34	103.00
1	A	175	ILE	N-CA-C	-6.59	98.01	107.77
1	A	172	LYS	N-CA-C	-6.47	105.03	113.12
1	A	174	ILE	CB-CA-C	5.78	119.47	111.38
1	A	222	ASP	N-CA-CB	-5.67	101.17	110.40
1	B	278	ILE	N-CA-C	-5.41	105.44	113.39

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 ⓘ

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	4207	62	0
1	B	4304	0	4254	80	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	13	0	10	4	0
3	B	13	0	10	3	0
4	A	423	0	0	0	0
4	B	417	0	0	0	1
All	All	9534	0	8543	144	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 (144) 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:216:CYS:HG	1:A:247:TRP:CG	1.90	0.89
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
1:B:219:ARG:HG3	1:B:220:LYS:N	2.04	0.70
1:A:79:GLU:HB2	1:A:220:LYS:C	2.16	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:86:LEU:HD21	1:A:212:LEU:HD13	1.77	0.65
3:A:602:CH9:HAH	3:A:602:CH9:OAA	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:B:72:VAL:HG21	1:B:243:MET:HE2	1.82	0.62
1:A:94:ILE:HD11	1:A:428:LEU:CD1	2.30	0.61
1:A:55:MET:HE3	1:A:64:GLU:HG3	1.83	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:204:ILE:HD11	1:B:290:ILE:HG22	1.85	0.57
1:B:219:ARG:HE	1:B:224:TYR:HE1	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:207:GLU:CD	1:A:289:PRO:HG2	2.30	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:OD1	1:A:248:ASN:N	2.39	0.55
1:A:70:LEU:O	1:A:245:ARG:NH2	2.39	0.55
1:A:252:CYS:SG	1:A:277:ILE:HD13	2.46	0.55
1:B:80:HIS:HE1	1:B:225:TRP:CD1	2.26	0.54
1:B:219:ARG:NE	1:B:224:TYR:HE1	2.05	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:B:227:PHE:HD1	1:B:238:VAL:HG12	1.76	0.51
1:B:271:LYS:HZ3	1:B:285:VAL:HG22	1.75	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:A:243:MET:SD	1:A:243:MET:C	2.94	0.49
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:B:225:TRP:CH2	1:B:321:MET:HE1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:TRP:CD1	2:A:601:FAD:HO2A	2.34	0.46
1:A:227:PHE:CZ	1:A:381:VAL:HG11	2.50	0.46
1:B:225:TRP:HH2	1:B:321:MET:HE1	1.81	0.46
1:B:220:LYS:CD	1:B:247:TRP:HZ2	2.29	0.45
1:B:247:TRP:HE3	1:B:250:TRP:CH2	2.35	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:86:LEU:HB3	1:B:278:ILE:O	2.17	0.44
1:A:7:THR:O	1:A:171:ALA:HA	2.17	0.44
1:A:42:SER:OG	1:A:46:ARG:NH1	2.50	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: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:223:MET:HE1	3:B:602:CH9:CAI	2.47	0.43
1:B:246:PRO:HA	1:B:247:TRP:HA	1.54	0.43
1:B:223:MET:HE3	1:B:242:ARG:HB2	2.00	0.43
1:A:326:LEU:C	1:A:326:LEU:HD23	2.43	0.43
1:B:277:ILE:O	1:B:277:ILE:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:THR:HA	1:A:560:ILE:HD12	2.02	0.42
1:B:320:PRO:HG2	3:B:602:CH9:CAH	2.49	0.42
1:B:477:TRP:HB3	1:B:484:ARG:HG2	2.02	0.42
1:B:205:ASN:OD1	1:B:253:VAL:HG13	2.20	0.42
1:B:488:LEU:O	1:B:558:MET:HE1	2.20	0.42
1:A:79:GLU:C	1:A:221:GLY:CA	2.93	0.41
1:B:23:THR:HG23	1:B:134:ARG:HD2	2.02	0.41
1:A:45:PRO:HB2	1:A:242:ARG:NH2	2.34	0.41
1:A:154:VAL:HG21	1:A:174:ILE:CG1	2.44	0.41
1:B:86:LEU:HB2	1:B:278:ILE:HA	2.03	0.41
1:B:245:ARG:O	1:B:247:TRP:HA	2.21	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:94:ILE:CD1	1:A:428:LEU:HD12	2.46	0.41
1:A:115:TYR:OH	1:A:435:GLU:OE2	2.30	0.41
1:B:238:VAL:HG23	1:B:238:VAL:O	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:OD1	1:A:178:ASP:N	2.54	0.40
1:B:357:ASP:OD1	1:B:361:SER:OG	2.30	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%)	43 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	549/586 (94%)	523 (95%)	22 (4%)	4 (1%)	18	23
All	All	1093/1172 (93%)	1048 (96%)	40 (4%)	5 (0%)	24	31

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 ⓘ

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%)	433 (98%)	10 (2%)	44	63
1	B	448/467 (96%)	441 (98%)	7 (2%)	55	73
All	All	891/934 (95%)	874 (98%)	17 (2%)	50	69

All (17) 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	238	VAL
1	A	248	ASN
1	A	277	ILE
1	A	319	THR
1	A	484	ARG
1	A	555	ARG
1	B	224	TYR

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Mol	Chain	Res	Type
1	B	276	GLU
1	B	282	GLU
1	B	285	VAL
1	B	483	ARG
1	B	484	ARG
1	B	495	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	186	GLN
1	A	509	HIS
1	A	531	GLN
1	B	80	HIS
1	B	147	HIS
1	B	186	GLN
1	B	509	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	3.67	7 (50%)	18,18,18	0.54	0
3	CH9	A	602	-	14,14,14	3.60	7 (50%)	18,18,18	0.97	1 (5%)
2	FAD	B	601	-	58,58,58	1.91	11 (18%)	85,89,89	2.00	19 (22%)
2	FAD	A	601	-	58,58,58	1.86	11 (18%)	85,89,89	2.02	21 (24%)

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	12/34/50/50	0/6/6/6
2	FAD	A	601	-	1/1/9/9	12/34/50/50	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C1'-C2'	7.04	1.62	1.52
2	A	601	FAD	C1'-C2'	6.43	1.61	1.52
3	B	602	CH9	CAC-CAH	6.23	1.49	1.38
3	A	602	CH9	CAE-CAG	6.12	1.49	1.38
3	B	602	CH9	CAE-CAG	6.11	1.49	1.38
3	B	602	CH9	CAF-CAJ	6.02	1.49	1.38
3	A	602	CH9	CAC-CAH	6.02	1.49	1.38
3	A	602	CH9	CAF-CAJ	5.99	1.49	1.38
2	B	601	FAD	C2'-C3'	5.21	1.62	1.53
3	B	602	CH9	CAD-CAB	5.12	1.49	1.38
2	B	601	FAD	C5X-N5	5.08	1.48	1.39
3	B	602	CH9	CAI-CAL	5.03	1.49	1.39
2	A	601	FAD	C5X-N5	4.96	1.48	1.39
3	A	602	CH9	CAD-CAB	4.94	1.49	1.38
3	A	602	CH9	CAI-CAL	4.86	1.49	1.39
2	A	601	FAD	C2'-C3'	4.52	1.61	1.53
2	B	601	FAD	C2-N1	4.20	1.46	1.36
2	A	601	FAD	C2-N1	4.03	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C6A-N6A	3.67	1.43	1.34
2	B	601	FAD	C6A-N6A	3.62	1.43	1.34
3	B	602	CH9	CAM-CAK	3.49	1.50	1.40
2	A	601	FAD	C5A-N7A	-3.26	1.33	1.39
3	A	602	CH9	CAM-CAK	3.11	1.49	1.40
2	B	601	FAD	C5A-N7A	-2.92	1.33	1.39
2	A	601	FAD	O2'-C2'	2.60	1.48	1.43
2	B	601	FAD	O2'-C2'	2.49	1.48	1.43
2	B	601	FAD	C4X-C10	2.46	1.51	1.44
3	A	602	CH9	CAJ-CAM	-2.43	1.36	1.40
2	A	601	FAD	O2B-C2B	-2.37	1.37	1.43
3	B	602	CH9	CAJ-CAM	-2.25	1.36	1.40
2	B	601	FAD	O2B-C2B	-2.23	1.37	1.43
2	B	601	FAD	O3B-C3B	-2.19	1.37	1.43
2	A	601	FAD	O4B-C4B	-2.16	1.40	1.45
2	B	601	FAD	O3'-C3'	-2.15	1.37	1.43
2	A	601	FAD	C4X-C10	2.13	1.50	1.44
2	A	601	FAD	O3B-C3B	-2.07	1.37	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	O2P-P-O3P	7.11	126.49	107.27
2	B	601	FAD	O2P-P-O3P	6.68	125.33	107.27
2	B	601	FAD	N3A-C2A-N1A	-6.24	119.14	128.58
2	A	601	FAD	N3A-C2A-N1A	-5.94	119.58	128.58
2	A	601	FAD	O2P-P-O5'	-5.58	82.26	107.57
2	B	601	FAD	O2P-P-O5'	-5.51	82.57	107.57
2	B	601	FAD	O5'-P-O1P	-5.10	88.71	108.94
2	A	601	FAD	O5'-P-O1P	-4.67	90.44	108.94
2	B	601	FAD	C5A-C4A-N3A	-4.12	121.05	126.72
2	A	601	FAD	C5A-N7A-C8A	3.99	109.73	103.45
2	A	601	FAD	C5A-C4A-N3A	-3.95	121.28	126.72
2	B	601	FAD	C5A-N7A-C8A	3.80	109.42	103.45
2	B	601	FAD	C2A-N3A-C4A	3.48	120.32	111.83
2	B	601	FAD	N3A-C4A-N9A	3.47	133.06	127.17
2	B	601	FAD	C4'-C3'-C2'	3.42	119.25	113.57
2	A	601	FAD	N3A-C4A-N9A	3.39	132.93	127.17
2	A	601	FAD	C5'-C4'-C3'	3.38	118.60	112.22
2	A	601	FAD	O2'-C2'-C3'	3.38	117.16	109.25
2	A	601	FAD	N9A-C8A-N7A	-3.32	109.22	113.94
2	B	601	FAD	N9A-C8A-N7A	-3.26	109.31	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C2A-N3A-C4A	3.20	119.66	111.83
2	A	601	FAD	C4A-C5A-N7A	-3.02	107.13	110.58
2	B	601	FAD	O2'-C2'-C3'	2.98	116.21	109.25
2	B	601	FAD	C4A-C5A-N7A	-2.95	107.21	110.58
3	A	602	CH9	CAL-CAM-CAK	-2.83	119.67	122.31
2	A	601	FAD	C4-C4X-N5	2.81	122.09	118.21
2	A	601	FAD	O3'-C3'-C4'	2.80	115.30	108.93
2	B	601	FAD	C1'-C2'-C3'	2.73	117.07	109.66
2	A	601	FAD	O4-C4-C4X	-2.71	119.37	126.53
2	A	601	FAD	C4'-C3'-C2'	2.71	118.08	113.57
2	B	601	FAD	C4-N3-C2	-2.70	120.85	125.64
2	A	601	FAD	C4-N3-C2	-2.67	120.91	125.64
2	A	601	FAD	C4X-C4-N3	2.56	119.77	113.25
2	B	601	FAD	C4X-C4-N3	2.46	119.53	113.25
2	B	601	FAD	C5'-C4'-C3'	2.46	116.85	112.22
2	A	601	FAD	C2A-N1A-C6A	2.43	122.73	118.73
2	B	601	FAD	C4A-N9A-C8A	2.31	108.16	105.74
2	B	601	FAD	C2A-N1A-C6A	2.29	122.49	118.73
2	A	601	FAD	C4A-N9A-C8A	2.28	108.13	105.74
2	B	601	FAD	O4-C4-C4X	-2.27	120.55	126.53
2	A	601	FAD	C10-C4X-N5	-2.13	120.45	124.81

All (2) chirality outliers are listed below:

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

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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'

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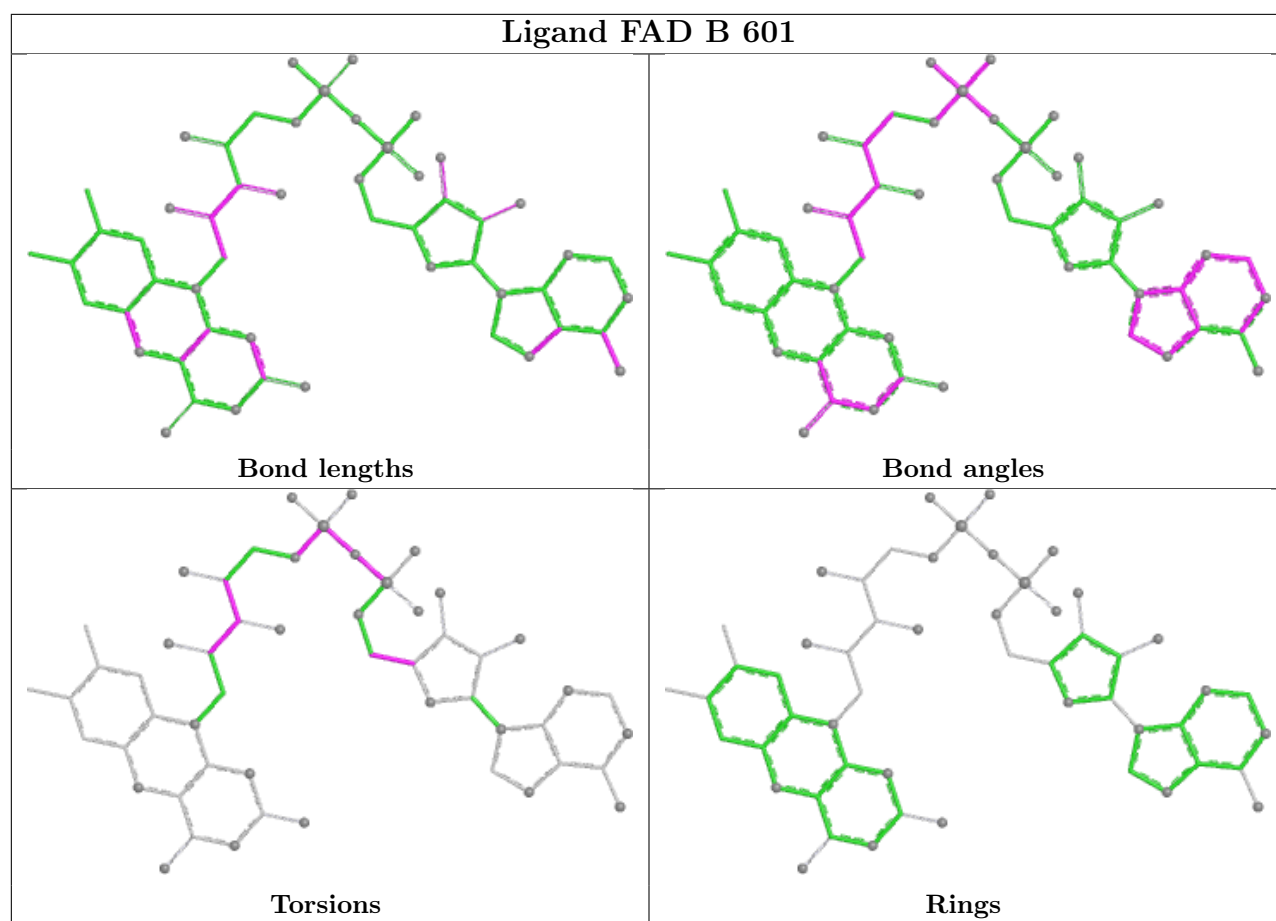
Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-C5'
3	A	602	CH9	CAH-CAL-CAM-CAJ
3	A	602	CH9	CAI-CAL-CAM-CAJ
3	A	602	CH9	CAH-CAL-CAM-CAK
2	A	601	FAD	P-O3P-PA-O5B
2	B	601	FAD	P-O3P-PA-O5B
2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

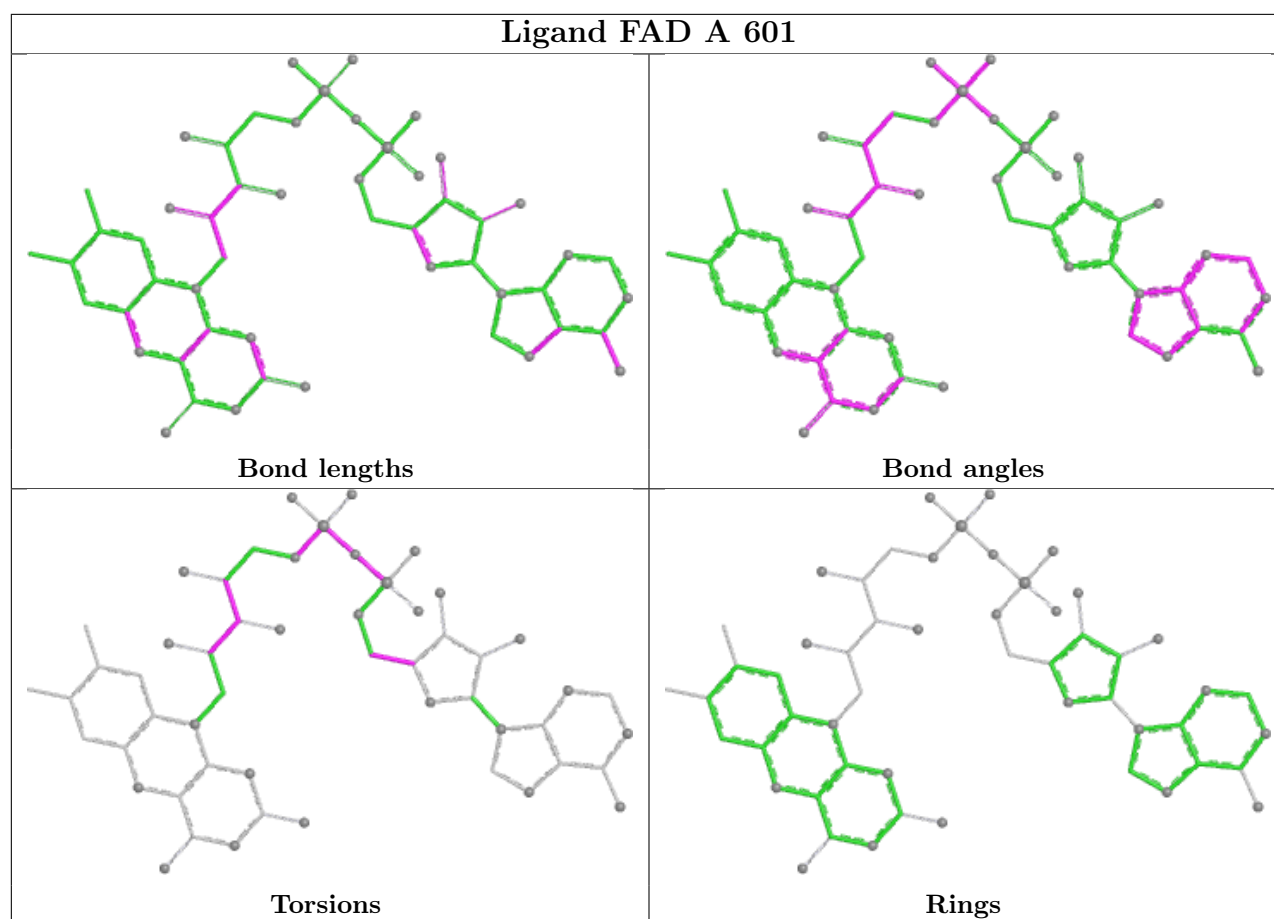
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	CH9	3	0
3	A	602	CH9	4	0
2	B	601	FAD	1	0
2	A	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%)	1.04	97 (17%) 4 4	12, 25, 78, 136	0
1	B	559/586 (95%)	0.96	98 (17%) 4 4	10, 25, 80, 142	0
All	All	1113/1172 (94%)	1.00	195 (17%) 4 4	10, 25, 80, 142	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	LEU	10.5
1	A	221	GLY	8.8
1	B	216	CYS	8.7
1	A	213	SER	8.5
1	B	243	MET	8.4
1	A	282	GLU	8.2
1	B	249	LYS	7.5
1	A	237	GLY	7.4
1	B	265	ILE	7.1
1	B	215	LEU	7.0
1	B	248	ASN	7.0
1	A	247	TRP	7.0
1	B	217	GLU	6.6
1	A	283	ILE	6.6
1	B	212	LEU	6.6
1	A	285	VAL	6.5
1	A	211	ASP	6.5
1	A	151	GLN	6.5
1	B	202	GLY	6.4
1	B	219	ARG	6.4
1	A	210	ALA	6.3
1	B	255	GLY	6.3
1	A	218	HIS	6.3
1	B	247	TRP	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	249	LYS	6.1
1	A	255	GLY	6.1
1	A	86	LEU	5.8
1	B	218	HIS	5.6
1	B	282	GLU	5.6
1	B	263	PRO	5.6
1	A	209	SER	5.6
1	A	270	ALA	5.5
1	B	250	TRP	5.4
1	A	284	PRO	5.4
1	A	389	PRO	5.3
1	A	276	GLU	5.3
1	B	214	SER	5.2
1	A	215	LEU	5.2
1	B	278	ILE	5.2
1	B	266	THR	5.1
1	B	196	MET	5.1
1	B	393	GLU	5.1
1	B	273	ILE	5.1
1	B	269	GLU	4.9
1	A	243	MET	4.9
1	A	483	ARG	4.9
1	A	286	GLU	4.8
1	B	195	GLN	4.8
1	A	248	ASN	4.7
1	A	278	ILE	4.7
1	B	238	VAL	4.6
1	A	38	TRP	4.6
1	B	210	ALA	4.5
1	B	271	LYS	4.5
1	A	274	ILE	4.5
1	A	246	PRO	4.4
1	A	244	ILE	4.4
1	B	275	HIS	4.4
1	B	570	GLU	4.4
1	B	87	ALA	4.4
1	B	390	ALA	4.4
1	A	222	ASP	4.4
1	B	222	ASP	4.4
1	A	250	TRP	4.4
1	B	39	ARG	4.4
1	B	211	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	225	TRP	4.4
1	A	224	TYR	4.3
1	A	217	GLU	4.3
1	A	275	HIS	4.3
1	A	238	VAL	4.3
1	B	209	SER	4.3
1	A	271	LYS	4.3
1	A	214	SER	4.3
1	A	281	ASP	4.3
1	B	283	ILE	4.3
1	B	254	TRP	4.2
1	B	285	VAL	4.2
1	A	202	GLY	4.2
1	B	392	THR	4.0
1	A	391	PRO	4.0
1	A	239	ALA	4.0
1	A	387	LEU	3.9
1	A	266	THR	3.9
1	B	201	SER	3.9
1	B	86	LEU	3.9
1	B	220	LYS	3.9
1	B	244	ILE	3.8
1	B	387	LEU	3.8
1	B	268	GLU	3.8
1	B	286	GLU	3.7
1	A	273	ILE	3.7
1	A	268	GLU	3.7
1	B	264	GLU	3.7
1	A	346	GLY	3.7
1	A	242	ARG	3.7
1	A	5	ALA	3.7
1	A	267	LYS	3.7
1	B	270	ALA	3.6
1	A	254	TRP	3.6
1	B	224	TYR	3.6
1	A	251	ILE	3.6
1	B	227	PHE	3.6
1	B	38	TRP	3.5
1	B	394	SER	3.5
1	A	79	GLU	3.5
1	A	27	SER	3.5
1	B	284	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	287	VAL	3.4
1	A	392	THR	3.4
1	B	301	VAL	3.4
1	A	390	ALA	3.4
1	B	272	LYS	3.4
1	A	277	ILE	3.3
1	B	389	PRO	3.3
1	B	391	PRO	3.3
1	B	516	GLN	3.3
1	B	88	GLY	3.3
1	B	80	HIS	3.3
1	A	378	PHE	3.3
1	B	267	LYS	3.3
1	B	246	PRO	3.3
1	B	280	THR	3.3
1	A	174	ILE	3.2
1	A	388	PRO	3.2
1	B	483	ARG	3.2
1	B	481	ASN	3.2
1	A	43	PRO	3.2
1	A	522	LEU	3.1
1	A	225	TRP	3.1
1	A	37	ARG	3.1
1	B	242	ARG	3.1
1	A	516	GLN	3.0
1	B	151	GLN	3.0
1	A	379	PRO	3.0
1	B	274	ILE	3.0
1	A	280	THR	3.0
1	A	396	MET	3.0
1	B	239	ALA	3.0
1	A	301	VAL	3.0
1	B	277	ILE	3.0
1	B	346	GLY	3.0
1	A	394	SER	3.0
1	A	208	PHE	2.9
1	B	569	ARG	2.9
1	A	272	LYS	2.9
1	A	205	ASN	2.9
1	A	227	PHE	2.8
1	A	216	CYS	2.8
1	A	45	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	6	GLU	2.8
1	A	194	GLY	2.8
1	B	205	ASN	2.7
1	B	276	GLU	2.7
1	B	76	TYR	2.7
1	A	279	GLY	2.7
1	A	152	ASP	2.7
1	B	223	MET	2.6
1	A	382	PHE	2.6
1	B	95	PRO	2.6
1	A	291	SER	2.6
1	A	187	ASN	2.5
1	A	288	GLY	2.5
1	B	449	GLY	2.5
1	B	382	PHE	2.5
1	B	171	ALA	2.5
1	A	39	ARG	2.4
1	A	220	LYS	2.4
1	B	37	ARG	2.4
1	A	400	LEU	2.4
1	B	221	GLY	2.4
1	B	287	VAL	2.4
1	B	93	ARG	2.4
1	A	76	TYR	2.3
1	B	174	ILE	2.3
1	A	252	CYS	2.3
1	A	292	THR	2.3
1	B	252	CYS	2.2
1	B	44	GLY	2.2
1	B	378	PHE	2.2
1	A	481	ASN	2.2
1	B	129	SER	2.2
1	B	245	ARG	2.2
1	B	379	PRO	2.2
1	B	292	THR	2.2
1	A	401	VAL	2.2
1	A	44	GLY	2.1
1	A	569	ARG	2.1
1	A	393	GLU	2.1
1	A	290	ILE	2.1
1	B	152	ASP	2.1
1	B	281	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	122	TYR	2.1
1	B	89	GLU	2.0
1	B	94	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

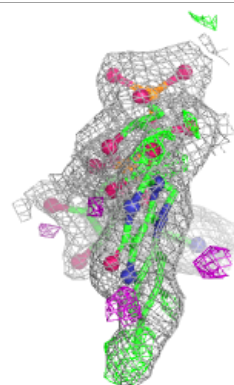
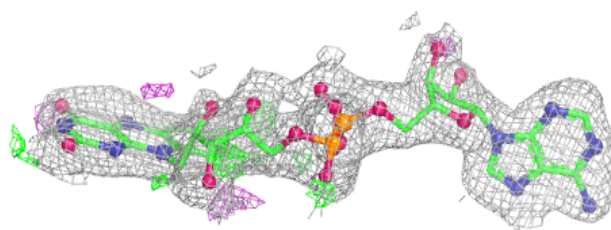
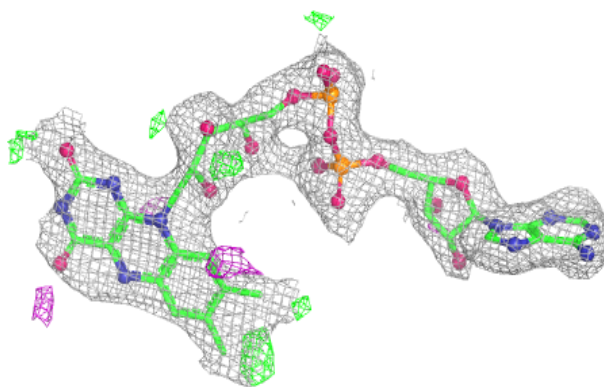
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CH9	B	602	13/13	0.79	0.21	59,63,64,65	0
3	CH9	A	602	13/13	0.84	0.20	58,60,64,64	0
2	FAD	A	601	53/53	0.92	0.12	20,31,41,46	0
2	FAD	B	601	53/53	0.92	0.11	17,27,43,47	0

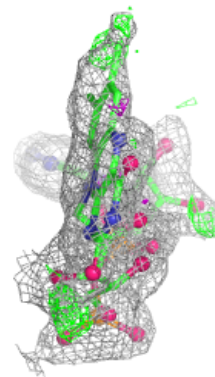
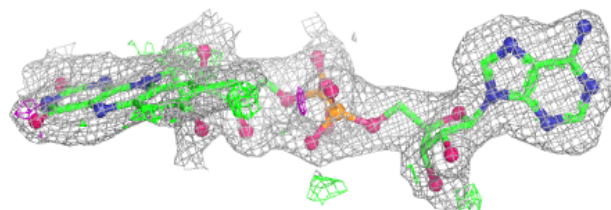
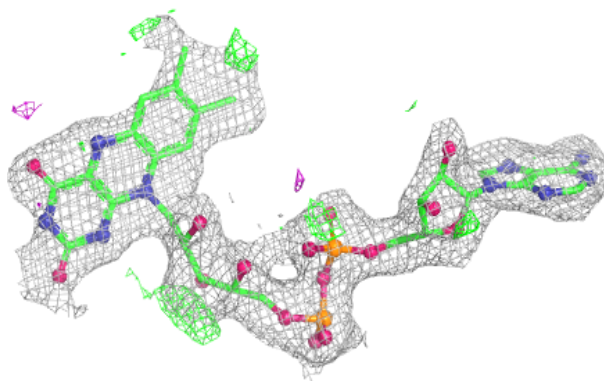
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

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.