



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:59 PM UTC

PDB ID : 1GV4 / pdb_00001gv4
Title : Murine apoptosis-inducing factor (AIF)
Authors : Mate, M.J.; Alzari, P.M.
Deposited on : 2002-02-05
Resolution : 2.00 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

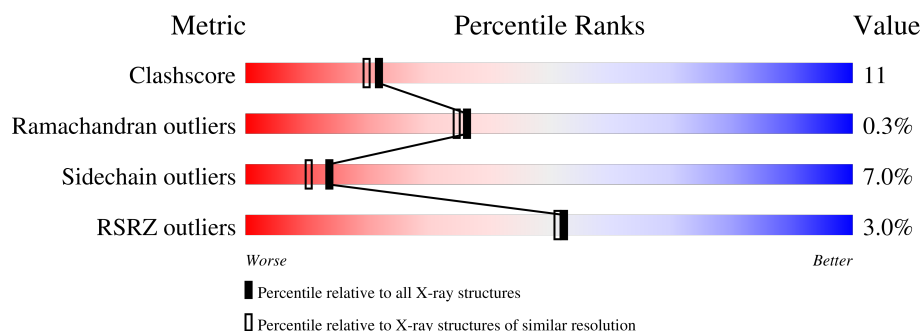
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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.

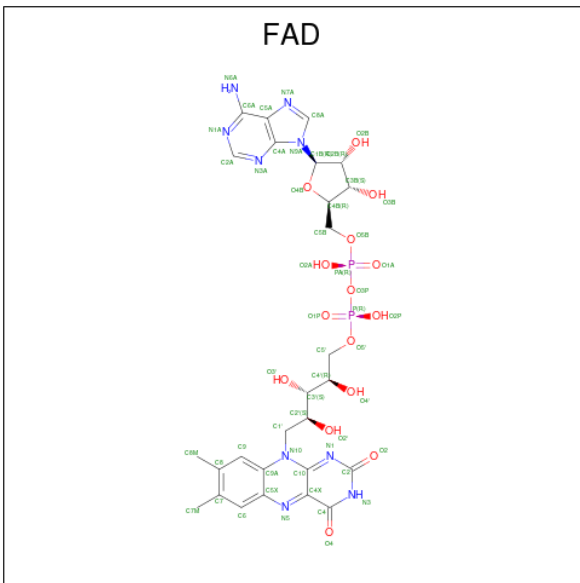
Mol	Chain	Length	Quality of chain
1	A	528	3% 72% 17% • • 7%
1	B	528	2% 71% 18% • • 7%

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 PROGRAMED CELL DEATH PROTEIN 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total 3759	C 2379	N 666	O 703	S 11	27	0	0
1	B	490	Total 3759	C 2379	N 666	O 703	S 11	37	0	0

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



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

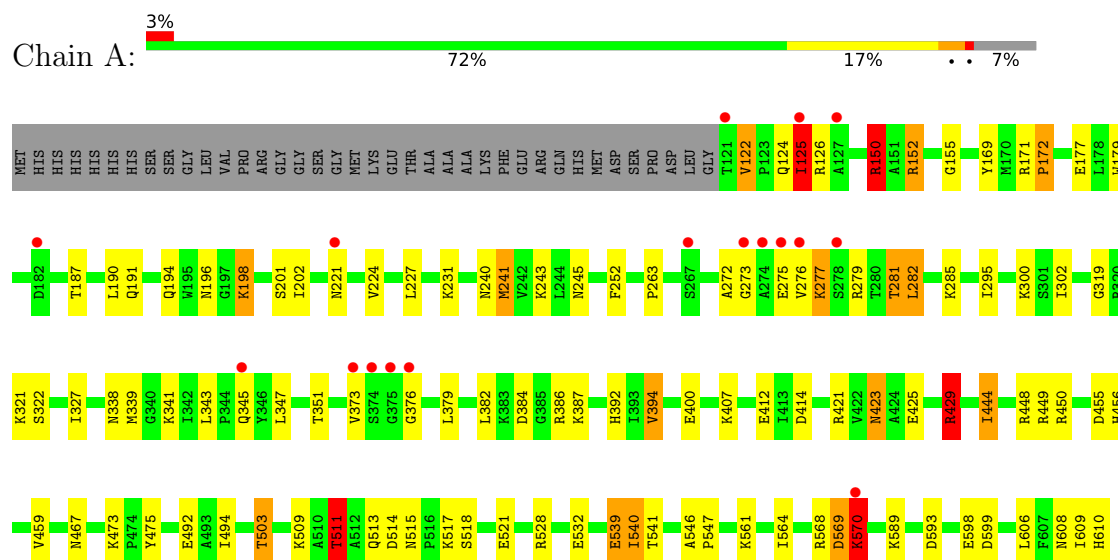
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total 214	O 214	0	0
3	B	226	Total 226	O 226	0	0

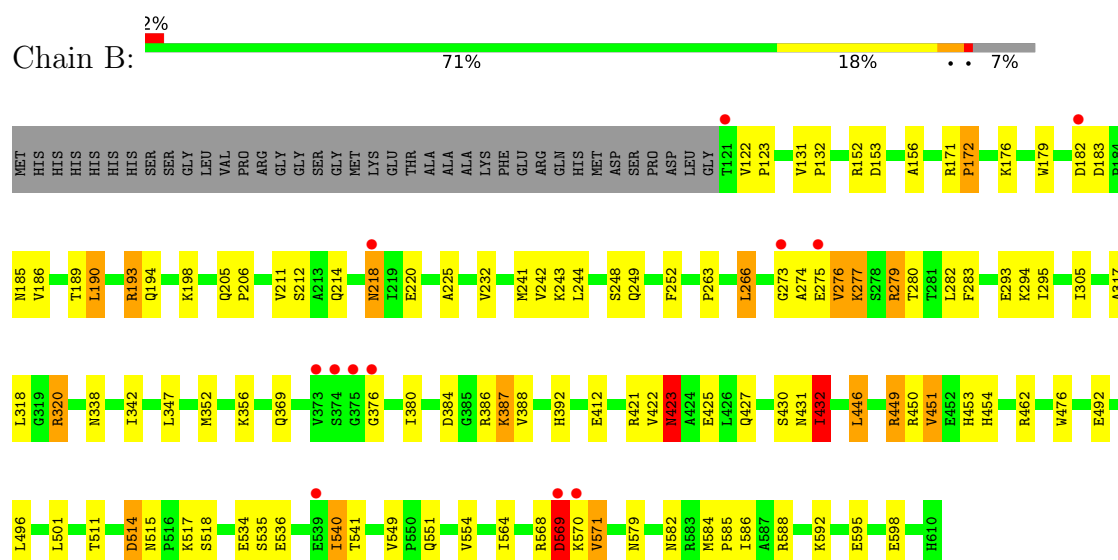
3 Residue-property plots

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: PROGRAMED CELL DEATH PROTEIN 8



• Molecule 1: PROGRAMED CELL DEATH PROTEIN 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.27Å 109.91Å 114.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 15.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (15.00-2.00) 95.9 (15.00-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.257 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8064	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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 51.19 % 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 5.8122e-05. 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: 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	0.97	2/3836 (0.1%)	1.16	14/5194 (0.3%)
1	B	1.10	3/3836 (0.1%)	1.29	33/5194 (0.6%)
All	All	1.03	5/7672 (0.1%)	1.23	47/10388 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	569	ASP	C-N	-32.34	0.87	1.33
1	B	568	ARG	C-N	18.68	1.59	1.33
1	A	539	GLU	CA-CB	-15.63	1.27	1.53
1	A	570	LYS	C-O	-7.50	1.14	1.24
1	B	176	LYS	CA-C	7.47	1.55	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	569	ASP	O-C-N	-30.02	82.67	122.59
1	B	569	ASP	CB-CA-C	13.00	136.29	110.42
1	B	569	ASP	CA-C-N	9.42	138.77	122.56
1	B	569	ASP	C-N-CA	9.42	138.77	122.56
1	A	277	LYS	CB-CG-CD	9.10	132.24	111.30
1	B	568	ARG	CA-C-N	-8.06	106.15	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	568	ARG	C-N-CA	-8.06	106.15	121.54
1	A	150	ARG	NE-CZ-NH1	-7.12	114.38	121.50
1	A	282	LEU	CA-C-N	-6.92	113.29	123.11
1	A	282	LEU	C-N-CA	-6.92	113.29	123.11
1	B	198	LYS	CB-CA-C	6.84	121.22	109.51
1	A	122	VAL	N-CA-CB	-6.76	104.43	111.87
1	B	294	LYS	N-CA-C	-6.68	104.08	111.36
1	B	214	GLN	CB-CA-C	-6.64	97.91	110.67
1	A	387	LYS	CB-CA-C	6.64	121.27	109.65
1	A	125	ILE	N-CA-CB	-6.63	103.30	110.53
1	B	432	ILE	CG1-CB-CG2	-6.63	90.82	110.70
1	B	275	GLU	CB-CA-C	6.47	121.16	110.81
1	A	394	VAL	CB-CA-C	-6.31	101.42	110.83
1	B	387	LYS	CB-CA-C	6.21	121.23	109.37
1	B	422	VAL	CA-C-N	6.17	133.32	121.54
1	B	422	VAL	C-N-CA	6.17	133.32	121.54
1	B	570	LYS	CB-CA-C	6.10	121.23	110.37
1	B	511	THR	N-CA-C	-6.08	101.20	110.14
1	B	182	ASP	N-CA-C	-6.06	106.53	114.04
1	B	283	PHE	N-CA-C	5.86	118.20	109.59
1	A	511	THR	N-CA-CB	-5.81	101.45	110.46
1	B	156	ALA	N-CA-C	5.79	118.41	110.24
1	B	571	VAL	N-CA-C	5.70	116.79	108.58
1	B	218	ASN	CA-C-N	-5.60	115.15	122.37
1	B	218	ASN	C-N-CA	-5.60	115.15	122.37
1	B	570	LYS	CA-C-O	5.53	126.13	119.43
1	B	595	GLU	CA-C-N	-5.50	115.11	122.42
1	B	595	GLU	C-N-CA	-5.50	115.11	122.42
1	B	276	VAL	CB-CA-C	-5.47	104.88	111.88
1	B	492	GLU	N-CA-C	-5.45	100.79	109.23
1	B	423	ASN	CB-CA-C	-5.39	99.70	110.42
1	B	598	GLU	CB-CA-C	5.37	121.20	109.99
1	A	429	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	B	172	PRO	N-CA-C	5.33	117.20	110.70
1	A	172	PRO	N-CA-C	5.32	117.19	110.70
1	B	514	ASP	N-CA-C	5.31	118.06	110.68
1	B	535	SER	N-CA-C	5.25	117.64	110.55
1	A	177	GLU	N-CA-C	5.17	117.58	111.33
1	A	150	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	B	369	GLN	N-CA-C	-5.01	106.86	113.12
1	A	539	GLU	N-CA-CB	5.01	119.32	111.56

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	569	ASP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	569	ASP	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	3759	0	3789	83	0
1	B	3759	0	3788	82	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
3	A	214	0	0	10	0
3	B	226	0	0	8	0
All	All	8064	0	7639	162	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 11.

All (162) 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:274:ALA:HA	1:B:277:LYS:CE	1.51	1.41
1:B:274:ALA:CA	1:B:277:LYS:HE2	1.49	1.37
1:A:272:ALA:HB1	1:A:276:VAL:HG21	1.44	0.98
1:B:273:GLY:O	1:B:277:LYS:HG3	1.64	0.97
1:B:421:ARG:NH2	3:B:2126:HOH:O	1.92	0.93
1:A:429:ARG:HD2	1:B:425:GLU:OE2	1.71	0.91
1:B:279:ARG:NH2	1:B:376:GLY:O	2.07	0.86
1:A:152:ARG:HG3	1:A:152:ARG:HH21	1.38	0.86
1:A:279:ARG:NH2	1:A:376:GLY:O	2.13	0.82
1:A:152:ARG:HG3	1:A:152:ARG:NH2	1.95	0.80
1:B:273:GLY:C	1:B:277:LYS:HD3	2.08	0.79
1:B:384:ASP:OD1	1:B:386:ARG:NH2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:THR:CG2	1:A:392:HIS:NE2	2.48	0.76
1:B:241:MET:HE1	1:B:243:LYS:HE3	1.68	0.76
1:B:273:GLY:O	1:B:277:LYS:CG	2.33	0.75
1:A:412:GLU:OE2	1:A:421:ARG:HD3	1.86	0.75
1:A:467:ASN:HD21	1:A:473:LYS:H	1.34	0.75
1:B:320:ARG:HH21	1:B:320:ARG:HG3	1.49	0.75
1:B:446:LEU:HD13	3:B:2210:HOH:O	1.85	0.75
1:A:570:LYS:O	3:A:2196:HOH:O	2.05	0.74
1:A:423:ASN:C	1:A:423:ASN:HD22	1.96	0.73
1:A:569:ASP:O	1:A:570:LYS:HB2	1.89	0.71
1:B:193:ARG:HH21	1:B:193:ARG:HG3	1.57	0.69
1:A:196:ASN:HD21	1:A:198:LYS:NZ	1.90	0.69
1:A:444:ILE:HG13	1:A:444:ILE:O	1.93	0.69
1:B:536:GLU:HG2	1:B:588:ARG:HB3	1.73	0.68
1:A:150:ARG:CD	3:A:2014:HOH:O	2.40	0.68
1:B:266:LEU:HD21	1:B:305:ILE:HG21	1.76	0.68
1:A:272:ALA:CB	1:A:276:VAL:HG21	2.21	0.66
1:B:183:ASP:HB3	1:B:186:VAL:HG23	1.75	0.66
1:A:517:LYS:O	1:A:521:GLU:HG3	1.96	0.65
1:B:276:VAL:O	1:B:280:THR:HG23	1.97	0.65
1:A:150:ARG:HD2	3:A:2014:HOH:O	1.96	0.65
1:A:421:ARG:HH11	1:A:448:ARG:HD2	1.62	0.64
1:A:155:GLY:HA2	1:A:221:ASN:O	1.98	0.64
1:A:569:ASP:O	1:A:570:LYS:CB	2.45	0.63
1:B:462:ARG:NH2	1:B:534:GLU:OE1	2.31	0.63
1:A:515:ASN:ND2	1:A:518:SER:H	1.96	0.63
1:A:272:ALA:HB1	1:A:276:VAL:CG2	2.26	0.63
1:B:273:GLY:O	1:B:277:LYS:CD	2.48	0.61
1:A:302:ILE:HG13	1:A:327:ILE:HD11	1.83	0.60
1:A:338:ASN:HD22	1:A:338:ASN:H	1.49	0.60
1:A:429:ARG:CD	1:B:425:GLU:OE2	2.45	0.60
1:A:467:ASN:ND2	1:A:473:LYS:H	1.99	0.60
1:A:196:ASN:HD21	1:A:198:LYS:HZ1	1.47	0.60
1:B:131:VAL:O	1:B:252:PHE:HA	2.01	0.60
1:A:414:ASP:HB2	1:A:421:ARG:HG3	1.84	0.60
1:A:152:ARG:HH21	1:A:152:ARG:CG	2.11	0.59
1:A:281:THR:HG22	1:A:392:HIS:NE2	2.16	0.59
1:A:382:LEU:HD12	1:A:386:ARG:HB2	1.84	0.59
1:B:384:ASP:OD2	1:B:386:ARG:HD3	2.04	0.58
1:A:150:ARG:HD3	3:A:2014:HOH:O	2.02	0.58
1:B:122:VAL:HB	1:B:123:PRO:CD	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ARG:HH21	1:B:320:ARG:CG	2.17	0.58
1:A:421:ARG:NH1	1:A:448:ARG:HD2	2.19	0.57
1:B:273:GLY:O	1:B:277:LYS:HD3	2.05	0.57
1:B:569:ASP:C	1:B:571:VAL:H	2.10	0.57
1:B:549:VAL:O	1:B:551:GLN:HG2	2.04	0.56
1:B:451:VAL:CG2	1:B:453:HIS:CE1	2.89	0.56
1:A:343:LEU:HD22	1:A:347:LEU:HD23	1.87	0.56
1:B:185:ASN:O	1:B:189:THR:HG23	2.06	0.56
1:B:274:ALA:C	1:B:277:LYS:HE2	2.27	0.55
1:B:449:ARG:HG3	1:B:450:ARG:N	2.19	0.55
1:B:122:VAL:HB	1:B:123:PRO:HD2	1.89	0.55
1:B:205:GLN:NE2	1:B:206:PRO:HD2	2.22	0.55
1:A:400:GLU:HG3	3:A:2108:HOH:O	2.06	0.54
1:A:423:ASN:ND2	1:A:425:GLU:H	2.06	0.54
1:A:339:MET:HE1	1:A:351:THR:HG21	1.90	0.54
1:A:540:ILE:O	1:A:540:ILE:HG22	2.08	0.54
1:A:231:LYS:H	1:A:245:ASN:HD22	1.54	0.54
1:B:427:GLN:NE2	3:B:2130:HOH:O	2.42	0.53
1:A:455:ASP:O	1:A:459:VAL:HG23	2.09	0.53
1:A:194:GLN:NE2	1:A:198:LYS:HE2	2.25	0.52
1:A:384:ASP:OD1	1:A:386:ARG:HD3	2.08	0.52
1:B:451:VAL:HG22	1:B:453:HIS:CE1	2.45	0.52
1:A:194:GLN:HE22	1:A:198:LYS:HE2	1.75	0.52
1:A:263:PRO:HB2	1:A:282:LEU:HB3	1.91	0.52
1:B:476:TRP:NE1	3:B:2167:HOH:O	2.40	0.51
1:B:263:PRO:HB2	1:B:282:LEU:HB3	1.92	0.51
1:A:179:TRP:O	1:A:321:LYS:HE2	2.10	0.51
1:A:423:ASN:C	1:A:423:ASN:ND2	2.66	0.50
1:A:241:MET:HE1	1:A:243:LYS:HE2	1.94	0.50
1:A:511:THR:HG23	1:A:513:GLN:H	1.76	0.50
1:B:193:ARG:HH21	1:B:193:ARG:CG	2.24	0.50
1:B:320:ARG:CG	1:B:320:ARG:NH2	2.73	0.50
1:B:412:GLU:OE1	1:B:421:ARG:HD3	2.11	0.50
1:A:528:ARG:HD3	3:A:2181:HOH:O	2.11	0.50
1:A:347:LEU:HD22	1:A:564:ILE:HD11	1.94	0.50
1:A:275:GLU:HB3	1:A:373:VAL:HG21	1.93	0.49
1:B:320:ARG:HG3	1:B:320:ARG:NH2	2.23	0.49
1:B:584:MET:N	1:B:585:PRO:CD	2.76	0.49
1:B:515:ASN:ND2	1:B:518:SER:H	2.11	0.49
1:A:568:ARG:O	1:A:569:ASP:HB2	2.12	0.48
1:B:540:ILE:HG22	1:B:541:THR:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ASN:HB3	1:B:425:GLU:H	1.78	0.48
1:A:589:LYS:HE3	1:A:593:ASP:OD2	2.14	0.48
1:A:191:GLN:HE22	1:A:201:SER:HB2	1.78	0.47
1:A:281:THR:HG23	1:A:392:HIS:NE2	2.29	0.47
1:A:241:MET:HE1	1:A:243:LYS:CE	2.45	0.47
1:A:503:THR:HG23	3:A:2098:HOH:O	2.14	0.47
1:B:347:LEU:HD22	1:B:564:ILE:HD11	1.95	0.47
1:B:430:SER:O	1:B:431:ASN:HB2	2.15	0.47
1:B:454:HIS:HD2	3:B:2007:HOH:O	1.96	0.47
1:B:536:GLU:HG2	1:B:588:ARG:CB	2.43	0.47
1:A:285:LYS:HE3	1:A:285:LYS:HB2	1.70	0.46
1:B:446:LEU:CD1	3:B:2210:HOH:O	2.54	0.46
1:B:277:LYS:HE3	1:B:277:LYS:HB2	1.68	0.46
1:B:384:ASP:CG	1:B:386:ARG:HH21	2.23	0.45
1:A:275:GLU:CB	1:A:373:VAL:HG21	2.45	0.45
1:A:319:GLY:O	1:A:322:SER:HB3	2.15	0.45
1:A:231:LYS:H	1:A:245:ASN:ND2	2.15	0.45
1:B:189:THR:O	1:B:190:LEU:HB2	2.16	0.45
1:A:429:ARG:HD3	1:B:425:GLU:HG3	1.99	0.45
1:A:171:ARG:N	1:A:172:PRO:CD	2.80	0.44
1:B:171:ARG:N	1:B:172:PRO:CD	2.80	0.44
1:B:449:ARG:HD3	3:B:2149:HOH:O	2.16	0.44
1:B:462:ARG:HH22	1:B:534:GLU:CD	2.26	0.44
1:A:608:ASN:OD1	1:A:610:HIS:HE1	2.00	0.44
1:B:446:LEU:HD11	1:B:496:LEU:HB2	2.00	0.44
1:B:515:ASN:ND2	1:B:517:LYS:HB3	2.33	0.44
1:B:514:ASP:HB3	1:B:579:ASN:O	2.17	0.44
1:A:546:ALA:HB1	1:A:547:PRO:HD2	2.00	0.43
1:A:540:ILE:HG12	1:A:589:LYS:HG3	1.99	0.43
1:B:352:MET:O	1:B:356:LYS:HG3	2.18	0.43
1:A:125:ILE:HA	3:A:2002:HOH:O	2.17	0.43
1:B:152:ARG:HA	1:B:152:ARG:HD3	1.69	0.43
1:A:240:ASN:HB3	1:A:252:PHE:O	2.19	0.43
1:A:273:GLY:O	1:A:276:VAL:HG22	2.19	0.43
1:B:432:ILE:HD13	1:B:432:ILE:HG23	1.07	0.43
1:A:503:THR:CG2	3:A:2098:HOH:O	2.67	0.43
1:A:492:GLU:OE1	1:A:532:GLU:OE1	2.37	0.42
1:B:295:ILE:HD13	1:B:392:HIS:CD2	2.54	0.42
1:B:347:LEU:HA	1:B:347:LEU:HD12	1.79	0.42
1:A:125:ILE:H	1:A:125:ILE:HG12	1.10	0.42
1:B:380:ILE:HB	1:B:388:VAL:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:VAL:O	1:B:225:ALA:HA	2.19	0.42
1:B:515:ASN:HD21	1:B:517:LYS:HB3	1.84	0.42
1:B:153:ASP:C	1:B:153:ASP:OD1	2.62	0.42
1:B:432:ILE:HD12	1:B:432:ILE:HG21	1.32	0.42
1:A:285:LYS:HD3	3:A:2019:HOH:O	2.20	0.41
1:A:456:HIS:HD2	1:A:475:TYR:OH	2.03	0.41
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.94	0.41
1:A:412:GLU:CD	1:A:421:ARG:HD3	2.45	0.41
1:B:243:LYS:HG2	1:B:249:GLN:HG2	2.03	0.41
1:B:338:ASN:HD22	1:B:338:ASN:H	1.69	0.41
1:A:150:ARG:HD2	1:A:224:VAL:HG23	2.02	0.41
1:A:169:TYR:HB2	1:A:202:ILE:HG12	2.03	0.41
1:A:561:LYS:HE3	1:A:609:ILE:HD13	2.02	0.41
1:A:421:ARG:NH1	1:B:421:ARG:HD2	2.36	0.41
1:B:179:TRP:CG	1:B:317:ALA:HB1	2.55	0.41
1:B:273:GLY:C	1:B:277:LYS:CD	2.85	0.41
1:A:511:THR:HG22	1:A:514:ASP:CG	2.46	0.40
1:A:276:VAL:HG23	1:A:277:LYS:N	2.35	0.40
1:A:295:ILE:HD13	1:A:392:HIS:CE1	2.55	0.40
1:B:232:VAL:HG13	1:B:242:VAL:HB	2.03	0.40
1:B:277:LYS:HG3	1:B:277:LYS:H	1.53	0.40
2:A:1611:FAD:H9	2:A:1611:FAD:H1'1	1.79	0.40
1:B:131:VAL:HA	1:B:132:PRO:HD3	1.90	0.40
1:B:193:ARG:CG	1:B:193:ARG:NH2	2.85	0.40
1:B:244:LEU:HD12	1:B:248:SER:OG	2.21	0.40
1:A:599:ASP:OD2	1:A:599:ASP:C	2.64	0.40
1:B:194:GLN:HB3	3:B:2032:HOH:O	2.20	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	488/528 (92%)	471 (96%)	15 (3%)	2 (0%)	30	27
1	B	488/528 (92%)	469 (96%)	18 (4%)	1 (0%)	43	42
All	All	976/1056 (92%)	940 (96%)	33 (3%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	ASP
1	A	570	LYS
1	B	569	ASP

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	402/432 (93%)	370 (92%)	32 (8%)	11	8
1	B	402/432 (93%)	378 (94%)	24 (6%)	17	14
All	All	804/864 (93%)	748 (93%)	56 (7%)	14	10

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	124	GLN
1	A	125	ILE
1	A	126	ARG
1	A	150	ARG
1	A	152	ARG
1	A	187	THR
1	A	190	LEU
1	A	198	LYS
1	A	227	LEU
1	A	241	MET
1	A	281	THR
1	A	300	LYS

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Mol	Chain	Res	Type
1	A	341	LYS
1	A	345	GLN
1	A	379	LEU
1	A	394	VAL
1	A	407	LYS
1	A	423	ASN
1	A	429	ARG
1	A	444	ILE
1	A	449	ARG
1	A	450	ARG
1	A	494	ILE
1	A	503	THR
1	A	509	LYS
1	A	511	THR
1	A	539	GLU
1	A	540	ILE
1	A	541	THR
1	A	598	GLU
1	A	606	LEU
1	B	190	LEU
1	B	193	ARG
1	B	212	SER
1	B	218	ASN
1	B	220	GLU
1	B	266	LEU
1	B	277	LYS
1	B	279	ARG
1	B	293	GLU
1	B	320	ARG
1	B	342	ILE
1	B	387	LYS
1	B	423	ASN
1	B	432	ILE
1	B	446	LEU
1	B	449	ARG
1	B	451	VAL
1	B	501	LEU
1	B	540	ILE
1	B	554	VAL
1	B	569	ASP
1	B	582	ASN
1	B	586	ILE

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Mol	Chain	Res	Type
1	B	592	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	194	GLN
1	A	196	ASN
1	A	205	GLN
1	A	245	ASN
1	A	323	GLN
1	A	338	ASN
1	A	345	GLN
1	A	402	ASN
1	A	423	ASN
1	A	453	HIS
1	A	456	HIS
1	A	467	ASN
1	A	478	GLN
1	A	515	ASN
1	A	522	GLN
1	A	551	GLN
1	A	610	HIS
1	B	205	GLN
1	B	221	ASN
1	B	338	ASN
1	B	392	HIS
1	B	427	GLN
1	B	431	ASN
1	B	454	HIS
1	B	515	ASN
1	B	522	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	FAD	B	1611	-	58,58,58	1.21	7 (12%)	85,89,89	1.68	20 (23%)
2	FAD	A	1611	-	58,58,58	1.10	5 (8%)	85,89,89	1.65	20 (23%)

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	1611	-	-	2/34/50/50	0/6/6/6
2	FAD	A	1611	-	-	2/34/50/50	0/6/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1611	FAD	C4X-N5	3.56	1.38	1.30
2	B	1611	FAD	C4X-N5	3.52	1.38	1.30
2	B	1611	FAD	C5'-C4'	3.06	1.56	1.51
2	B	1611	FAD	C2A-N3A	2.95	1.39	1.33
2	A	1611	FAD	C5A-N7A	-2.87	1.33	1.39
2	A	1611	FAD	C10-N1	2.60	1.38	1.33
2	B	1611	FAD	C10-N1	2.54	1.38	1.33
2	B	1611	FAD	C5A-N7A	-2.44	1.34	1.39
2	A	1611	FAD	C2A-N1A	2.29	1.38	1.33
2	B	1611	FAD	C2A-N1A	2.22	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1611	FAD	C2A-N3A	2.22	1.37	1.33
2	B	1611	FAD	O2B-C2B	-2.01	1.38	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1611	FAD	N3A-C2A-N1A	-6.27	119.08	128.58
2	A	1611	FAD	N3A-C2A-N1A	-4.20	122.22	128.58
2	B	1611	FAD	C5A-C4A-N3A	-4.07	121.11	126.72
2	A	1611	FAD	N9A-C8A-N7A	-4.05	108.19	113.94
2	A	1611	FAD	O4'-C4'-C5'	-3.80	101.60	109.99
2	B	1611	FAD	C4X-C10-N10	3.62	121.66	116.48
2	B	1611	FAD	O3P-PA-O1A	-3.50	100.17	110.70
2	A	1611	FAD	C5A-N7A-C8A	3.44	108.86	103.45
2	A	1611	FAD	C9A-C5X-N5	-3.42	118.82	122.45
2	B	1611	FAD	C2A-N3A-C4A	3.22	119.70	111.83
2	A	1611	FAD	C5A-C4A-N3A	-3.12	122.42	126.72
2	A	1611	FAD	C4-N3-C2	-2.92	120.45	125.64
2	A	1611	FAD	C5X-C9A-N10	2.91	120.60	117.97
2	B	1611	FAD	N9A-C8A-N7A	-2.89	109.84	113.94
2	B	1611	FAD	O2P-P-O3P	-2.87	99.51	107.27
2	B	1611	FAD	C4-N3-C2	-2.83	120.61	125.64
2	A	1611	FAD	O3B-C3B-C4B	-2.76	103.17	111.08
2	A	1611	FAD	C4X-C4-N3	2.72	120.19	113.25
2	B	1611	FAD	C5A-N7A-C8A	2.72	107.72	103.45
2	A	1611	FAD	C4X-C10-N10	2.62	120.23	116.48
2	B	1611	FAD	C4-C4X-N5	2.54	121.72	118.21
2	B	1611	FAD	C4X-C4-N3	2.52	119.67	113.25
2	B	1611	FAD	C10-C4X-N5	-2.43	119.84	124.81
2	A	1611	FAD	C4A-C5A-N7A	-2.42	107.82	110.58
2	A	1611	FAD	C10-C4X-N5	-2.40	119.91	124.81
2	A	1611	FAD	C10-N1-C2	2.38	122.01	116.85
2	B	1611	FAD	C5X-C9A-N10	2.38	120.12	117.97
2	B	1611	FAD	N3A-C4A-N9A	2.33	131.12	127.17
2	A	1611	FAD	O4-C4-C4X	-2.31	120.44	126.53
2	B	1611	FAD	C4A-C5A-N7A	-2.30	107.95	110.58
2	A	1611	FAD	C6A-C5A-C4A	2.28	120.29	117.18
2	B	1611	FAD	C2A-N1A-C6A	2.19	122.33	118.73
2	B	1611	FAD	O5B-C5B-C4B	-2.17	101.61	108.99
2	A	1611	FAD	C4-C4X-N5	2.17	121.20	118.21
2	B	1611	FAD	C10-N1-C2	2.16	121.53	116.85
2	A	1611	FAD	C4X-C10-N1	-2.14	119.33	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1611	FAD	O4B-C1B-C2B	-2.13	102.06	106.62
2	A	1611	FAD	O4'-C4'-C3'	2.09	114.14	109.25
2	B	1611	FAD	C5B-C4B-C3B	-2.07	107.77	115.21
2	A	1611	FAD	C5X-N5-C4X	2.01	121.34	118.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

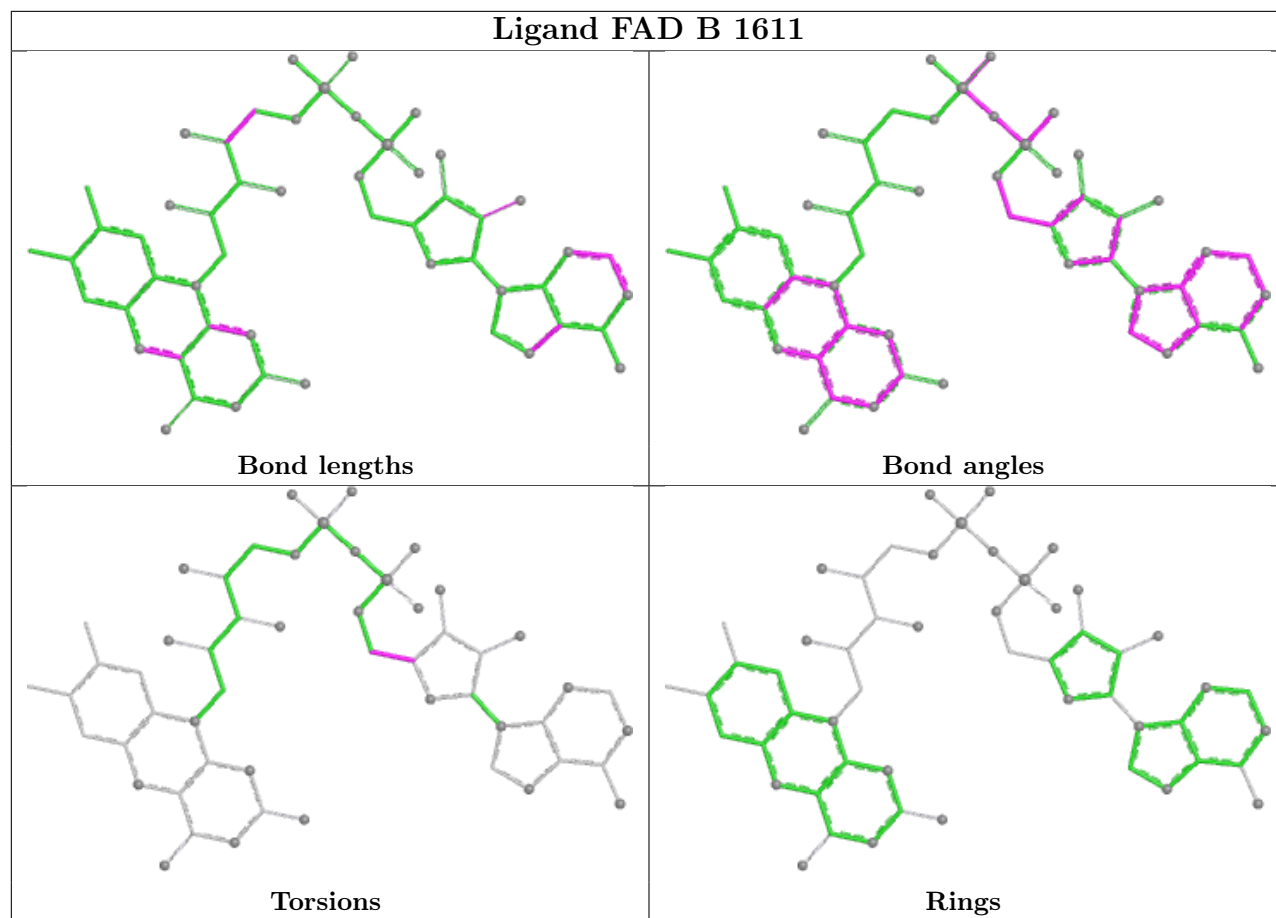
Mol	Chain	Res	Type	Atoms
2	A	1611	FAD	O4B-C4B-C5B-O5B
2	A	1611	FAD	C3B-C4B-C5B-O5B
2	B	1611	FAD	O4B-C4B-C5B-O5B
2	B	1611	FAD	C3B-C4B-C5B-O5B

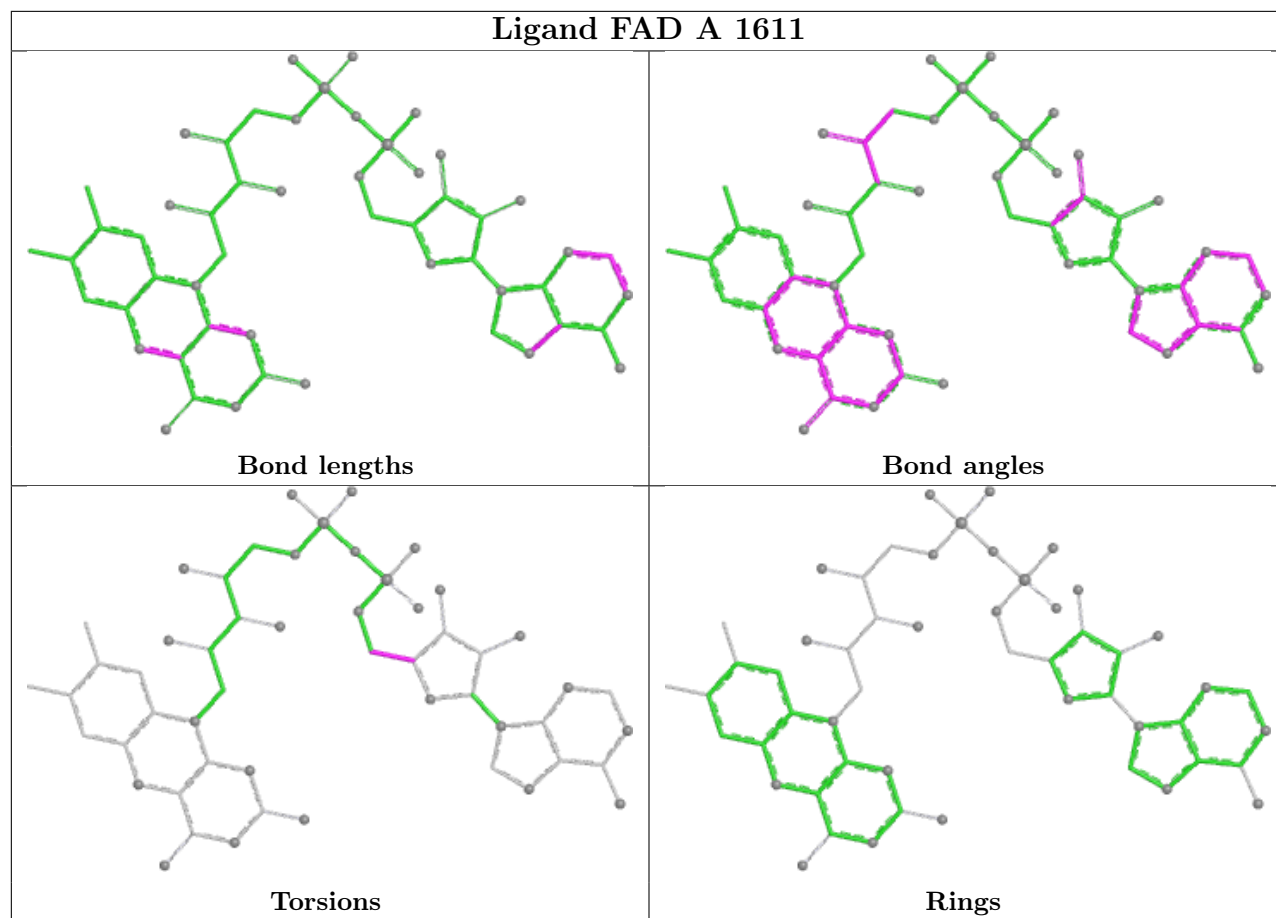
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1611	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	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	569:ASP	C	570:LYS	N	0.87

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	490/528 (92%)	0.13	17 (3%)	47 46	6, 13, 22, 30	6 (1%)
1	B	490/528 (92%)	0.17	12 (2%)	59 59	7, 13, 23, 30	9 (1%)
All	All	980/1056 (92%)	0.15	29 (2%)	52 51	6, 13, 23, 30	15 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	539	GLU	6.6
1	A	570	LYS	4.8
1	B	121	THR	4.1
1	A	373	VAL	4.0
1	A	273	GLY	3.6
1	B	275	GLU	3.3
1	B	569	ASP	3.1
1	B	182	ASP	3.0
1	A	125	ILE	3.0
1	A	275	GLU	2.8
1	B	273	GLY	2.8
1	B	376	GLY	2.7
1	A	182	ASP	2.6
1	A	127	ALA	2.6
1	A	121	THR	2.5
1	A	376	GLY	2.5
1	A	274	ALA	2.5
1	B	374	SER	2.5
1	A	278	SER	2.4
1	A	375	GLY	2.3
1	A	221	ASN	2.3
1	B	218	ASN	2.2
1	B	570	LYS	2.2
1	A	267	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	276	VAL	2.1
1	B	373	VAL	2.1
1	B	375	GLY	2.1
1	A	374	SER	2.1
1	A	345	GLN	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](#)

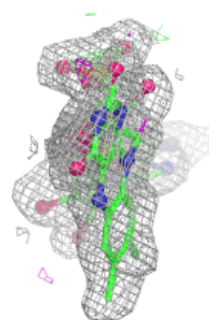
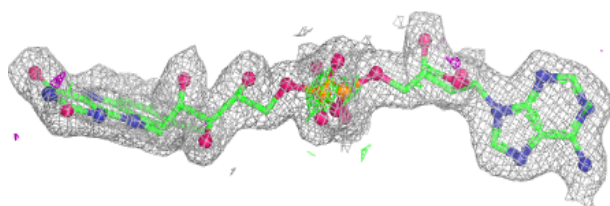
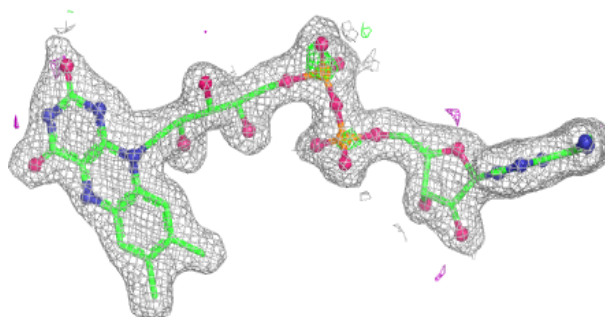
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	1611	53/53	0.95	0.09	12,16,19,26	0
2	FAD	B	1611	53/53	0.95	0.09	13,17,22,25	0

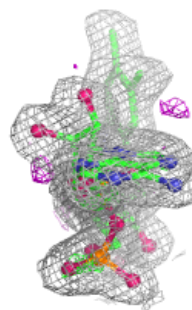
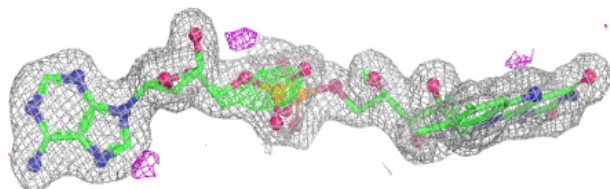
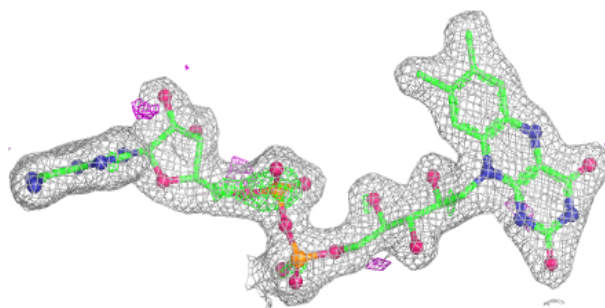
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 1611:

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

**Electron density around FAD B 1611:**

$2mF_o-DF_c$ (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.