



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:07 AM UTC

PDB ID : 3WE0 / pdb_00003we0
Title : L-Amino acid oxidase/monooxygenase from Pseudomonas sp. AIU 813
Authors : Im, D.H.; Matsui, D.; Fukuta, Y.; Fushinobu, S.; Isobe, K.; Asano, Y.
Deposited on : 2013-06-26
Resolution : 1.90 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

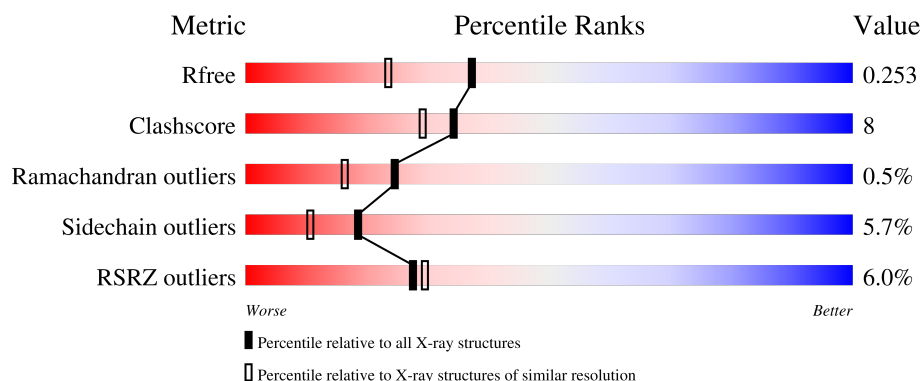
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	580	4% 76% 15% 7%
1	B	580	7% 74% 17% 7%

2 Entry composition [i](#)

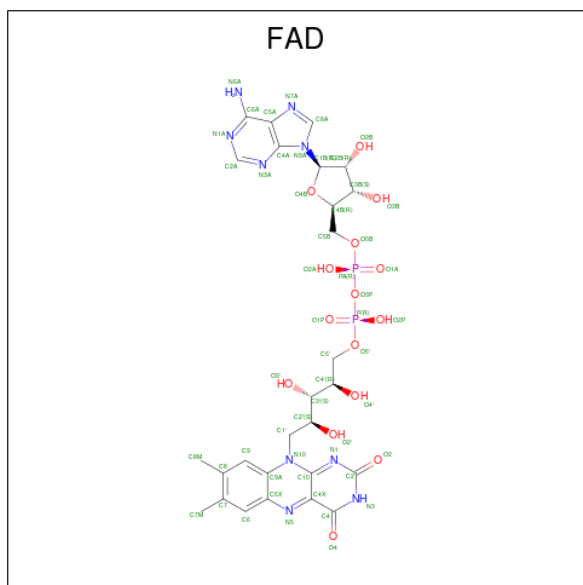
There are 3 unique types of molecules in this entry. The entry contains 8986 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-amino acid oxidase/monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4238	2706	732	779	21			
1	B	540	Total	C	N	O	S	0	0	0
			4238	2706	732	779	21			

- 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	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		

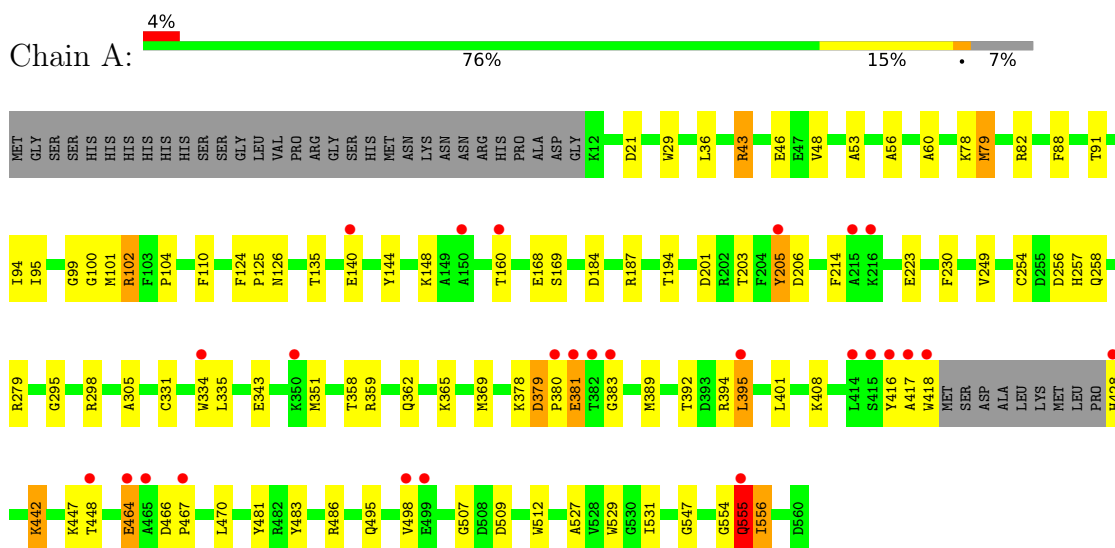
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	218	Total 218	O 218	0	0
3	B	186	Total 186	O 186	0	0

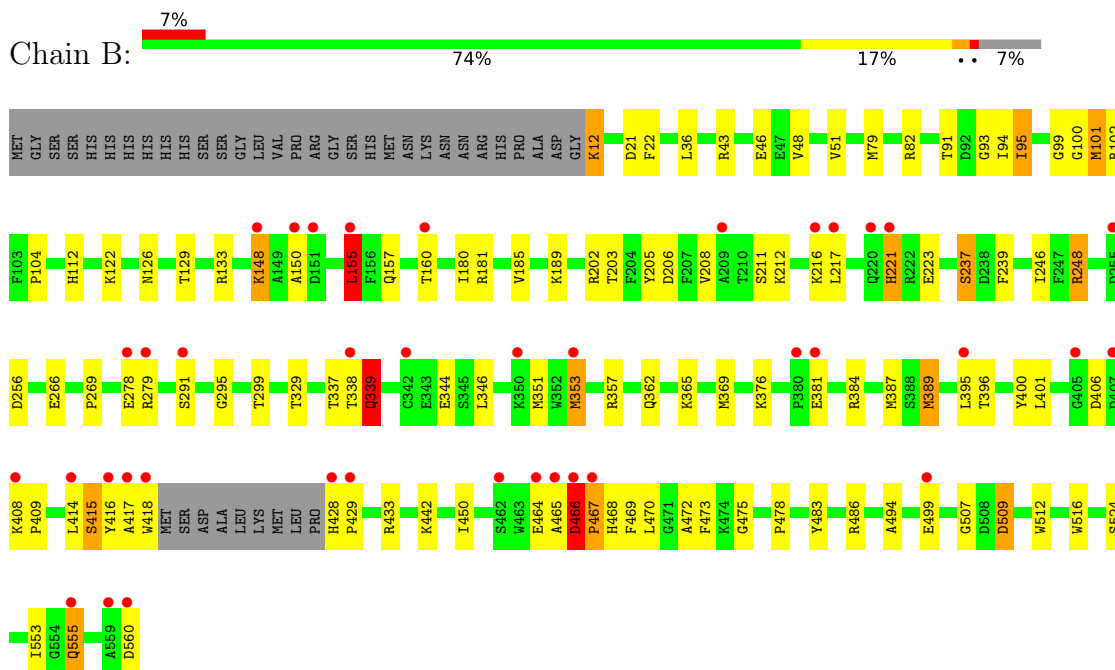
3 Residue-property plots [i](#)

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: L-amino acid oxidase/monooxygenase



- Molecule 1: L-amino acid oxidase/monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.93Å 141.35Å 75.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.38 – 1.90 30.38 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.38-1.90) 97.0 (30.38-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.209 , 0.254 0.209 , 0.253	Depositor DCC
R_{free} test set	5044 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8986	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.44	15/4359 (0.3%)	1.25	12/5925 (0.2%)
1	B	1.46	21/4359 (0.5%)	1.27	22/5925 (0.4%)
All	All	1.45	36/8718 (0.4%)	1.26	34/11850 (0.3%)

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	0	1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	553	ILE	N-CA	7.74	1.54	1.46
1	A	555	GLN	C-O	-7.11	1.14	1.23
1	B	266	GLU	C-O	6.37	1.32	1.24
1	A	104	PRO	C-O	6.35	1.31	1.23
1	B	414	LEU	N-CA	6.24	1.54	1.46
1	B	507	GLY	C-O	6.11	1.29	1.23
1	B	509	ASP	N-CA	5.95	1.53	1.46
1	B	185	VAL	CA-C	5.85	1.58	1.52
1	B	516	TRP	CA-C	-5.85	1.45	1.52
1	B	524	SER	C-O	5.75	1.30	1.24
1	B	417	ALA	CA-C	5.75	1.59	1.52
1	A	56	ALA	N-CA	5.68	1.53	1.46
1	A	126	ASN	C-O	-5.61	1.16	1.23
1	A	110	PHE	N-CA	5.59	1.53	1.46
1	B	104	PRO	C-O	5.57	1.30	1.23
1	B	126	ASN	C-O	-5.54	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	ILE	N-CA	5.53	1.53	1.46
1	A	168	GLU	CD-OE1	5.47	1.35	1.25
1	A	60	ALA	C-O	-5.45	1.17	1.24
1	A	507	GLY	C-O	5.41	1.27	1.23
1	B	494	ALA	N-CA	5.38	1.52	1.46
1	B	180	ILE	N-CA	5.32	1.52	1.46
1	A	53	ALA	CA-C	5.31	1.59	1.53
1	A	29	TRP	CD2-CE2	5.30	1.50	1.41
1	B	239	PHE	CA-C	5.29	1.59	1.52
1	A	144	TYR	CA-C	-5.19	1.46	1.52
1	B	384	ARG	N-CA	5.19	1.52	1.45
1	B	155	LEU	CA-C	5.17	1.59	1.52
1	A	135	THR	CA-C	-5.16	1.46	1.52
1	A	531	ILE	C-O	5.12	1.29	1.24
1	B	269	PRO	CA-CB	5.11	1.61	1.53
1	B	221	HIS	CG-CD2	5.10	1.41	1.35
1	B	112	HIS	ND1-CE1	5.06	1.37	1.32
1	B	555	GLN	C-O	-5.03	1.18	1.23
1	A	214	PHE	N-CA	5.03	1.52	1.46
1	A	556	ILE	C-O	-5.02	1.18	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	ASP	CA-C-N	-9.59	107.85	119.84
1	B	466	ASP	C-N-CA	-9.59	107.85	119.84
1	A	205	TYR	CB-CA-C	-7.20	99.47	110.92
1	A	295	GLY	N-CA-C	6.94	121.91	113.79
1	A	509	ASP	CB-CA-C	-6.57	98.06	110.67
1	A	79	MET	CG-SD-CE	-6.49	86.63	100.90
1	B	389	MET	N-CA-C	-6.44	100.51	110.10
1	B	208	VAL	N-CA-C	6.22	116.96	110.62
1	B	248	ARG	NE-CZ-NH2	6.15	124.73	119.20
1	B	291	SER	CB-CA-C	-6.08	101.25	110.92
1	B	299	THR	CA-C-N	6.08	125.88	120.10
1	B	299	THR	C-N-CA	6.08	125.88	120.10
1	A	527	ALA	N-CA-C	5.83	117.63	111.28
1	B	101	MET	CG-SD-CE	-5.78	88.19	100.90
1	B	468	HIS	N-CA-C	5.76	127.13	111.00
1	A	169	SER	N-CA-C	5.75	117.23	111.07
1	B	256	ASP	N-CA-C	5.74	116.13	108.38
1	B	248	ARG	NE-CZ-NH1	-5.59	115.91	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	417	ALA	N-CA-C	5.51	116.89	108.52
1	B	129	THR	CA-C-N	5.48	125.82	119.47
1	B	129	THR	C-N-CA	5.48	125.82	119.47
1	B	475	GLY	N-CA-C	-5.45	102.37	110.71
1	A	379	ASP	CA-C-N	5.42	125.50	119.32
1	A	379	ASP	C-N-CA	5.42	125.50	119.32
1	A	554	GLY	O-C-N	-5.33	117.10	122.59
1	B	295	GLY	N-CA-C	5.33	121.08	114.37
1	B	346	LEU	N-CA-C	5.21	117.87	111.82
1	A	417	ALA	N-CA-C	5.21	118.09	109.85
1	B	466	ASP	C-N-CD	-5.13	103.97	125.00
1	B	122	LYS	N-CA-C	5.10	114.17	108.25
1	A	43	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	A	389	MET	N-CA-C	-5.06	102.57	110.10
1	B	93	GLY	N-CA-C	5.03	121.70	114.10
1	B	509	ASP	CB-CA-C	-5.02	101.34	110.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	415	SER	Peptide

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	4238	0	4091	56	0
1	B	4238	0	4091	77	0
2	A	53	0	31	3	0
2	B	53	0	31	2	0
3	A	218	0	0	2	0
3	B	186	0	0	3	0
All	All	8986	0	8244	128	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 8.

All (128) 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:22:PHE:HB2	1:B:555:GLN:OE1	1.25	1.26
1:B:94:ILE:HG21	1:B:369:MET:HE3	1.26	1.08
1:A:94:ILE:HG21	1:A:369:MET:HE2	1.11	1.08
1:B:91:THR:HG21	1:B:369:MET:HE1	1.33	1.06
1:B:467:PRO:HA	1:B:469:PHE:H	1.22	1.03
1:A:94:ILE:HG21	1:A:369:MET:CE	1.91	1.00
1:A:94:ILE:CG2	1:A:369:MET:HE2	1.94	0.97
1:B:362:GLN:OE1	1:B:464:GLU:HG3	1.67	0.94
1:A:362:GLN:OE1	1:A:464:GLU:HG3	1.68	0.93
1:A:464:GLU:CD	1:A:464:GLU:H	1.77	0.90
1:B:94:ILE:HG21	1:B:369:MET:CE	2.01	0.90
1:B:94:ILE:CG2	1:B:369:MET:HE3	2.02	0.89
1:A:94:ILE:CG2	1:A:369:MET:CE	2.51	0.87
1:B:338:THR:O	1:B:339:GLN:HB2	1.74	0.85
1:B:101:MET:HE2	1:B:416:TYR:HE2	1.41	0.84
1:B:486:ARG:HD2	3:B:747:HOH:O	1.77	0.83
1:A:555:GLN:NE2	1:A:555:GLN:H	1.75	0.82
1:B:555:GLN:NE2	1:B:555:GLN:H	1.75	0.82
1:B:101:MET:HE2	1:B:416:TYR:CE2	2.14	0.81
1:B:22:PHE:CB	1:B:555:GLN:OE1	2.20	0.81
1:B:467:PRO:HA	1:B:469:PHE:N	1.96	0.80
1:A:378:LYS:HE3	1:A:383:GLY:O	1.84	0.78
1:A:91:THR:HG21	1:A:369:MET:HE1	1.68	0.75
1:B:133:ARG:HH21	1:B:376:LYS:HE2	1.50	0.74
1:B:387:MET:HE1	1:B:450:ILE:HD13	1.69	0.72
1:A:362:GLN:OE1	1:A:362:GLN:HA	1.90	0.72
1:B:133:ARG:HE	1:B:376:LYS:HG2	1.52	0.72
1:B:512:TRP:CZ2	1:B:555:GLN:HG2	2.24	0.72
1:B:202:ARG:NH2	1:B:206:ASP:OD2	2.22	0.71
1:B:338:THR:O	1:B:339:GLN:CB	2.39	0.71
1:B:95:ILE:HD12	1:B:95:ILE:C	2.16	0.71
1:A:486:ARG:HD2	3:A:740:HOH:O	1.90	0.70
1:A:256:ASP:OD2	1:A:257:HIS:ND1	2.22	0.69
1:A:362:GLN:OE1	1:A:464:GLU:CG	2.41	0.69
1:B:465:ALA:O	1:B:466:ASP:HB3	1.91	0.68
1:B:101:MET:CE	1:B:416:TYR:HE2	2.07	0.66
1:B:21:ASP:HB3	1:B:555:GLN:HG3	1.79	0.64
1:B:43:ARG:NH1	1:B:46:GLU:OE1	2.31	0.64
1:A:362:GLN:CD	1:A:464:GLU:HG3	2.22	0.64
1:B:465:ALA:O	1:B:466:ASP:CB	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:THR:OG1	1:B:205:TYR:HB2	1.97	0.63
1:B:101:MET:CE	1:B:416:TYR:CE2	2.80	0.63
1:B:217:LEU:HB3	1:B:221:HIS:ND1	2.14	0.63
1:A:555:GLN:H	1:A:555:GLN:CD	2.06	0.62
1:B:155:LEU:HD12	1:B:221:HIS:CD2	2.34	0.62
1:B:387:MET:HE1	1:B:450:ILE:CD1	2.30	0.62
1:B:512:TRP:HZ2	1:B:555:GLN:HG2	1.66	0.61
1:B:21:ASP:OD2	1:B:248:ARG:HD3	2.01	0.61
1:B:155:LEU:CD1	1:B:221:HIS:HD2	2.14	0.60
1:B:555:GLN:H	1:B:555:GLN:CD	2.09	0.59
1:B:157:GLN:O	1:B:160:THR:HG22	2.03	0.59
1:B:418:TRP:CZ3	1:B:473:PHE:CZ	2.91	0.59
1:A:223:GLU:OE2	1:B:483:TYR:OH	2.20	0.59
1:A:512:TRP:HZ2	1:A:555:GLN:HG3	1.69	0.58
1:B:362:GLN:CD	1:B:464:GLU:HG3	2.29	0.58
1:A:88:PHE:CD2	1:A:369:MET:HE3	2.40	0.57
1:A:100:GLY:HA2	2:A:601:FAD:C5X	2.36	0.56
1:A:395:LEU:CD1	1:A:395:LEU:H	2.19	0.55
1:A:464:GLU:CD	1:A:464:GLU:N	2.58	0.55
1:B:387:MET:CE	1:B:450:ILE:HD11	2.38	0.54
1:A:95:ILE:C	1:A:95:ILE:HD12	2.33	0.54
1:A:203:THR:OG1	1:A:205:TYR:HB2	2.07	0.54
1:B:12:LYS:HE3	1:B:181:ARG:CZ	2.37	0.54
1:B:387:MET:CE	1:B:450:ILE:CD1	2.85	0.53
1:A:101:MET:HE2	1:A:416:TYR:CE2	2.44	0.52
1:B:387:MET:HE3	1:B:450:ILE:HD11	1.90	0.52
1:A:249:VAL:HG13	1:A:254:CYS:HB2	1.91	0.52
1:B:12:LYS:HE3	1:B:181:ARG:NH2	2.25	0.52
1:A:331:CYS:HB2	1:A:335:LEU:HD12	1.91	0.52
1:A:483:TYR:OH	1:B:223:GLU:OE2	2.21	0.52
1:B:396:THR:O	1:B:416:TYR:O	2.29	0.51
1:B:466:ASP:O	1:B:467:PRO:CB	2.55	0.51
1:B:91:THR:CG2	1:B:369:MET:HE1	2.23	0.51
1:B:555:GLN:CD	1:B:555:GLN:N	2.68	0.51
1:A:512:TRP:CZ2	1:A:555:GLN:HG3	2.45	0.51
1:A:442:LYS:HE3	1:A:448:THR:O	2.10	0.50
1:A:395:LEU:H	1:A:395:LEU:HD13	1.76	0.50
1:B:353:MET:HE1	1:B:357:ARG:HH11	1.77	0.49
1:A:555:GLN:CD	1:A:555:GLN:N	2.68	0.49
1:A:82:ARG:O	1:A:99:GLY:HA3	2.13	0.49
1:B:100:GLY:HA2	2:B:601:FAD:C5X	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:CD1	1:B:221:HIS:CD2	2.94	0.48
1:A:206:ASP:OD2	1:B:206:ASP:HB2	2.12	0.48
1:A:100:GLY:HA2	2:A:601:FAD:N5	2.28	0.48
1:A:481:TYR:OH	1:A:555:GLN:HB2	2.14	0.48
1:A:184:ASP:OD2	1:A:187:ARG:NH2	2.44	0.48
1:A:102:ARG:HB2	1:A:258:GLN:HB3	1.95	0.48
1:B:338:THR:O	1:B:338:THR:OG1	2.30	0.47
1:B:466:ASP:O	1:B:467:PRO:HB3	2.14	0.47
1:A:124:PHE:CG	1:A:125:PRO:HD2	2.50	0.47
1:B:148:LYS:HB2	1:B:148:LYS:HE2	1.33	0.47
1:A:362:GLN:CD	1:A:464:GLU:CG	2.86	0.47
1:B:82:ARG:O	1:B:99:GLY:HA3	2.15	0.47
1:B:369:MET:HE2	1:B:409:PRO:CB	2.45	0.46
1:B:472:ALA:O	2:B:601:FAD:HM81	2.15	0.46
1:A:392:THR:HG23	1:A:394:ARG:N	2.30	0.46
1:A:529:TRP:CD2	1:A:547:GLY:HA3	2.51	0.46
3:A:825:HOH:O	1:B:223:GLU:HG2	2.15	0.46
1:B:429:PRO:O	1:B:433:ARG:HG3	2.15	0.46
1:B:365:LYS:HD2	1:B:416:TYR:CE1	2.50	0.45
1:B:95:ILE:C	1:B:95:ILE:CD1	2.89	0.45
1:A:392:THR:HG23	1:A:394:ARG:H	1.82	0.44
1:B:353:MET:CE	1:B:357:ARG:HH11	2.30	0.44
1:A:140:GLU:OE2	1:B:353:MET:HG2	2.18	0.44
1:B:509:ASP:HB2	3:B:862:HOH:O	2.18	0.43
1:A:334:TRP:HB3	1:A:470:LEU:HD13	2.01	0.43
1:B:237:SER:HB3	3:B:784:HOH:O	2.18	0.43
1:B:351:MET:SD	1:B:486:ARG:HG3	2.59	0.43
1:A:305:ALA:HA	1:A:343:GLU:HB2	1.99	0.43
1:B:51:VAL:HB	1:B:329:THR:HA	2.01	0.42
1:A:379:ASP:HA	1:A:380:PRO:HD2	1.83	0.42
1:A:43:ARG:HD2	1:A:46:GLU:OE2	2.19	0.42
1:A:466:ASP:OD1	1:A:467:PRO:HD2	2.20	0.42
1:B:365:LYS:HA	1:B:415:SER:O	2.19	0.42
1:B:337:THR:C	1:B:338:THR:HG23	2.46	0.41
1:B:148:LYS:NZ	1:B:150:ALA:H	2.18	0.41
1:A:206:ASP:CG	1:B:206:ASP:HB2	2.45	0.41
1:A:21:ASP:HB3	1:A:555:GLN:OE1	2.20	0.41
1:A:351:MET:SD	1:A:486:ARG:HG3	2.61	0.41
1:A:358:THR:O	1:A:359:ARG:HD3	2.21	0.41
1:A:416:TYR:CE1	1:A:418:TRP:CZ2	3.09	0.41
1:A:529:TRP:CE3	1:A:547:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:HG2	2:A:601:FAD:O4	2.22	0.40
1:A:160:THR:OG1	1:A:230:PHE:HB2	2.21	0.40
1:B:337:THR:OG1	1:B:338:THR:HG23	2.22	0.40
1:B:365:LYS:HD2	1:B:416:TYR:CZ	2.56	0.40
1:B:389:MET:HE3	1:B:400:TYR:CE1	2.56	0.40
1:B:203:THR:HG22	1:B:478:PRO:HG3	2.04	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	536/580 (92%)	522 (97%)	13 (2%)	1 (0%)	43	36
1	B	536/580 (92%)	518 (97%)	14 (3%)	4 (1%)	18	10
All	All	1072/1160 (92%)	1040 (97%)	27 (2%)	5 (0%)	24	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	GLN
1	B	467	PRO
1	A	381	GLU
1	B	406	ASP
1	B	466	ASP

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	440/474 (93%)	417 (95%)	23 (5%)	21	13
1	B	440/474 (93%)	413 (94%)	27 (6%)	17	9
All	All	880/948 (93%)	830 (94%)	50 (6%)	18	11

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	48	VAL
1	A	78	LYS
1	A	79	MET
1	A	102	ARG
1	A	148	LYS
1	A	194	THR
1	A	201	ASP
1	A	279	ARG
1	A	298	ARG
1	A	365	LYS
1	A	381	GLU
1	A	395	LEU
1	A	401	LEU
1	A	408	LYS
1	A	428	HIS
1	A	442	LYS
1	A	447	LYS
1	A	464	GLU
1	A	495	GLN
1	A	498	VAL
1	A	555	GLN
1	A	556	ILE
1	B	12	LYS
1	B	36	LEU
1	B	48	VAL
1	B	79	MET
1	B	95	ILE
1	B	102	ARG
1	B	148	LYS
1	B	155	LEU
1	B	189	LYS
1	B	211	SER

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Mol	Chain	Res	Type
1	B	212	LYS
1	B	216	LYS
1	B	237	SER
1	B	278	GLU
1	B	279	ARG
1	B	339	GLN
1	B	344	GLU
1	B	353	MET
1	B	381	GLU
1	B	395	LEU
1	B	401	LEU
1	B	408	LYS
1	B	428	HIS
1	B	442	LYS
1	B	470	LEU
1	B	499	GLU
1	B	560	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	A	435	GLN
1	A	468	HIS
1	A	495	GLN
1	A	540	HIS
1	B	177	GLN
1	B	339	GLN
1	B	404	ASN
1	B	484	ASN
1	B	540	HIS
1	B	555	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	A	601	-	58,58,58	2.28	18 (31%)	85,89,89	2.07	24 (28%)
2	FAD	B	601	-	58,58,58	2.06	18 (31%)	85,89,89	2.05	31 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	601	-	-	3/34/50/50	0/6/6/6
2	FAD	B	601	-	-	1/34/50/50	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	PA-O3P	7.44	1.67	1.59
2	A	601	FAD	P-O3P	6.08	1.66	1.59
2	A	601	FAD	C9A-C5X	5.80	1.50	1.41
2	B	601	FAD	PA-O3P	5.59	1.65	1.59
2	B	601	FAD	C9A-C5X	5.24	1.49	1.41
2	A	601	FAD	C1'-C2'	-4.90	1.45	1.52
2	B	601	FAD	C5X-N5	-4.33	1.31	1.39
2	B	601	FAD	C8-C7	3.97	1.50	1.40
2	B	601	FAD	C5A-C4A	3.61	1.45	1.39
2	A	601	FAD	C2A-N3A	3.38	1.39	1.33
2	A	601	FAD	C4'-C3'	-3.22	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C5A-N7A	-3.12	1.33	1.39
2	B	601	FAD	C1'-N10	3.11	1.55	1.47
2	A	601	FAD	C5'-C4'	3.11	1.56	1.51
2	A	601	FAD	C8-C7	3.04	1.48	1.40
2	B	601	FAD	C9-C8	-3.04	1.35	1.39
2	B	601	FAD	C4-N3	-2.99	1.33	1.38
2	B	601	FAD	C1'-C2'	-2.78	1.48	1.52
2	B	601	FAD	C5A-C6A	2.78	1.48	1.41
2	A	601	FAD	C4-N3	-2.72	1.33	1.38
2	A	601	FAD	C5A-C6A	2.71	1.48	1.41
2	B	601	FAD	C4'-C3'	-2.67	1.48	1.53
2	B	601	FAD	C5A-N7A	-2.49	1.34	1.39
2	B	601	FAD	C2-N1	-2.45	1.31	1.36
2	B	601	FAD	C8A-N7A	2.38	1.36	1.31
2	A	601	FAD	C3B-C4B	2.37	1.59	1.53
2	A	601	FAD	C2A-N1A	2.37	1.38	1.33
2	A	601	FAD	C8A-N9A	-2.32	1.33	1.37
2	B	601	FAD	C4A-N9A	-2.28	1.32	1.37
2	B	601	FAD	C6-C7	-2.26	1.36	1.39
2	A	601	FAD	C7M-C7	2.25	1.55	1.51
2	A	601	FAD	C5A-C4A	2.22	1.43	1.39
2	A	601	FAD	C8A-N7A	2.21	1.35	1.31
2	B	601	FAD	C2A-N1A	2.20	1.37	1.33
2	A	601	FAD	C4X-N5	2.14	1.35	1.30
2	B	601	FAD	O4-C4	2.01	1.27	1.23

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	N3A-C2A-N1A	-7.42	117.35	128.58
2	B	601	FAD	N3A-C2A-N1A	-5.85	119.72	128.58
2	A	601	FAD	C2A-N1A-C6A	5.65	128.01	118.73
2	A	601	FAD	C9A-C5X-N5	-4.88	117.28	122.45
2	A	601	FAD	O3P-P-O1P	-4.71	96.53	110.70
2	B	601	FAD	C9A-C5X-N5	-4.65	117.52	122.45
2	B	601	FAD	C2A-N1A-C6A	4.30	125.79	118.73
2	A	601	FAD	C5A-N7A-C8A	4.12	109.92	103.45
2	B	601	FAD	C5A-C4A-N3A	-3.98	121.24	126.72
2	A	601	FAD	N9A-C8A-N7A	-3.88	108.43	113.94
2	B	601	FAD	C1'-C2'-C3'	-3.70	99.61	109.66
2	A	601	FAD	O3'-C3'-C4'	-3.70	100.52	108.93
2	B	601	FAD	C4A-C5A-N7A	-3.67	106.39	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4A-C5A-N7A	-3.55	106.52	110.58
2	B	601	FAD	O3P-P-O1P	-3.54	100.06	110.70
2	B	601	FAD	C7M-C7-C6	3.43	125.62	119.57
2	B	601	FAD	C2A-N3A-C4A	3.33	119.98	111.83
2	B	601	FAD	N9A-C8A-N7A	-3.27	109.30	113.94
2	A	601	FAD	C4A-N9A-C8A	3.24	109.14	105.74
2	B	601	FAD	C9-C8-C7	3.16	124.33	119.69
2	B	601	FAD	C5A-N7A-C8A	3.16	108.42	103.45
2	B	601	FAD	O2P-P-O1P	3.09	126.80	112.44
2	B	601	FAD	C4A-N9A-C8A	3.08	108.98	105.74
2	A	601	FAD	C2A-N3A-C4A	3.04	119.26	111.83
2	A	601	FAD	O4B-C1B-C2B	-3.01	100.18	106.62
2	A	601	FAD	O2A-PA-O1A	2.96	126.21	112.44
2	A	601	FAD	O2P-P-O1P	2.93	126.06	112.44
2	A	601	FAD	C5A-C4A-N3A	-2.90	122.72	126.72
2	B	601	FAD	O4-C4-C4X	-2.84	119.03	126.53
2	B	601	FAD	N3A-C4A-N9A	2.78	131.89	127.17
2	A	601	FAD	C5'-C4'-C3'	-2.73	107.07	112.22
2	B	601	FAD	C4-C4X-N5	2.61	121.82	118.21
2	B	601	FAD	C6-C5X-C9A	2.54	122.54	119.05
2	B	601	FAD	C6A-C5A-N7A	2.53	136.97	132.09
2	A	601	FAD	N3A-C4A-N9A	2.50	131.41	127.17
2	B	601	FAD	C5'-C4'-C3'	-2.50	107.51	112.22
2	B	601	FAD	C5X-N5-C4X	2.49	122.12	118.09
2	A	601	FAD	C4-C4X-N5	2.49	121.64	118.21
2	B	601	FAD	O3P-PA-O1A	-2.47	103.28	110.70
2	A	601	FAD	C2'-C1'-N10	2.43	121.69	110.20
2	A	601	FAD	O4-C4-C4X	-2.42	120.15	126.53
2	B	601	FAD	O4B-C1B-C2B	-2.39	101.49	106.62
2	A	601	FAD	C6A-C5A-N7A	2.38	136.67	132.09
2	B	601	FAD	O2A-PA-O1A	2.30	123.14	112.44
2	B	601	FAD	O4'-C4'-C5'	-2.26	105.00	109.99
2	B	601	FAD	C8M-C8-C7	-2.25	116.16	120.76
2	A	601	FAD	C9-C8-C7	2.21	122.94	119.69
2	B	601	FAD	C2'-C1'-N10	2.19	120.57	110.20
2	B	601	FAD	C5X-C9A-N10	2.18	119.94	117.97
2	A	601	FAD	O4'-C4'-C3'	-2.13	104.26	109.25
2	A	601	FAD	C10-N1-C2	2.11	121.42	116.85
2	B	601	FAD	C4X-C4-N3	2.09	118.57	113.25
2	B	601	FAD	C4X-C10-N1	-2.08	119.48	124.59
2	B	601	FAD	C1'-N10-C9A	2.05	124.61	120.63
2	A	601	FAD	C5X-N5-C4X	2.04	121.39	118.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

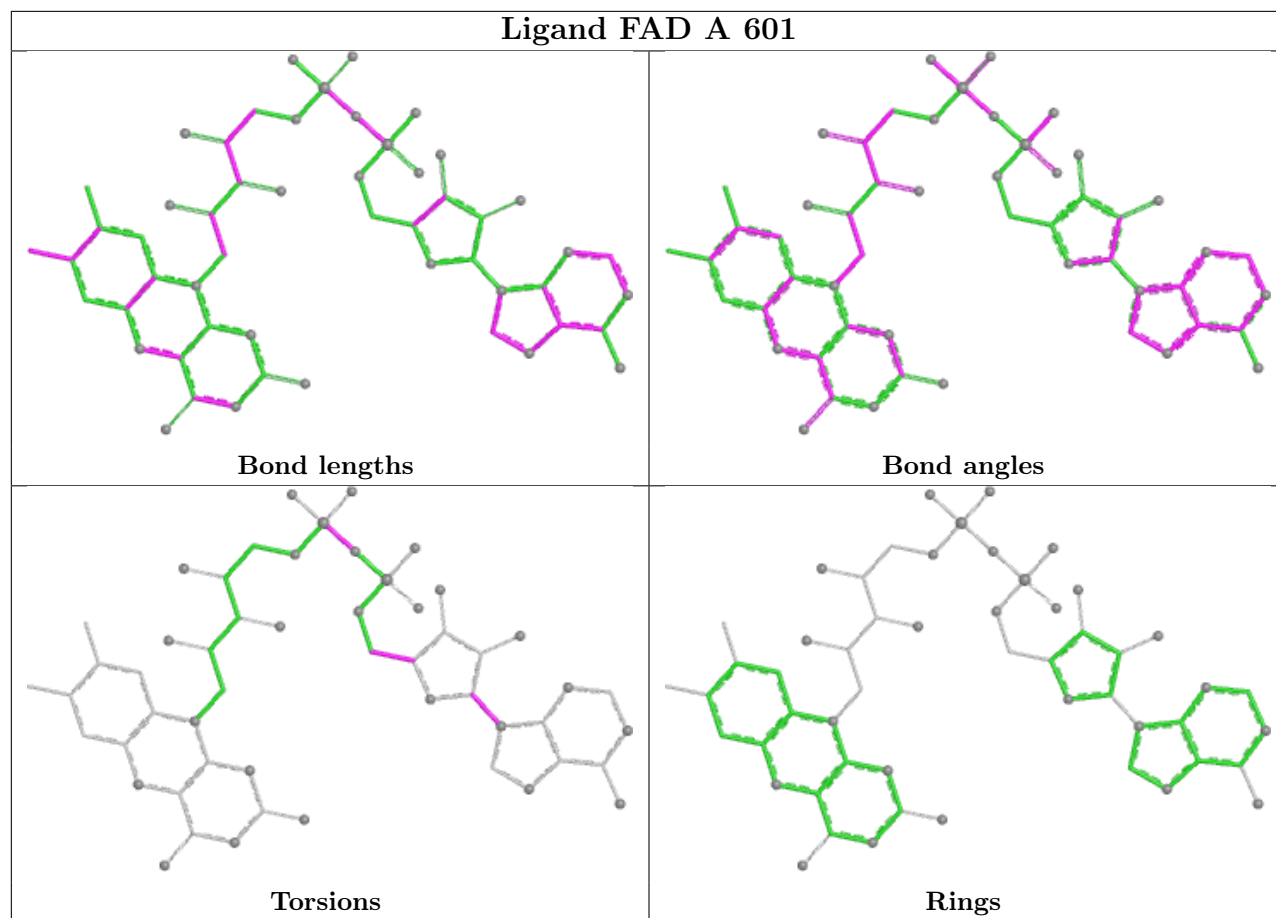
Mol	Chain	Res	Type	Atoms
2	B	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	PA-O3P-P-O5'
2	A	601	FAD	C2B-C1B-N9A-C8A
2	A	601	FAD	O4B-C4B-C5B-O5B

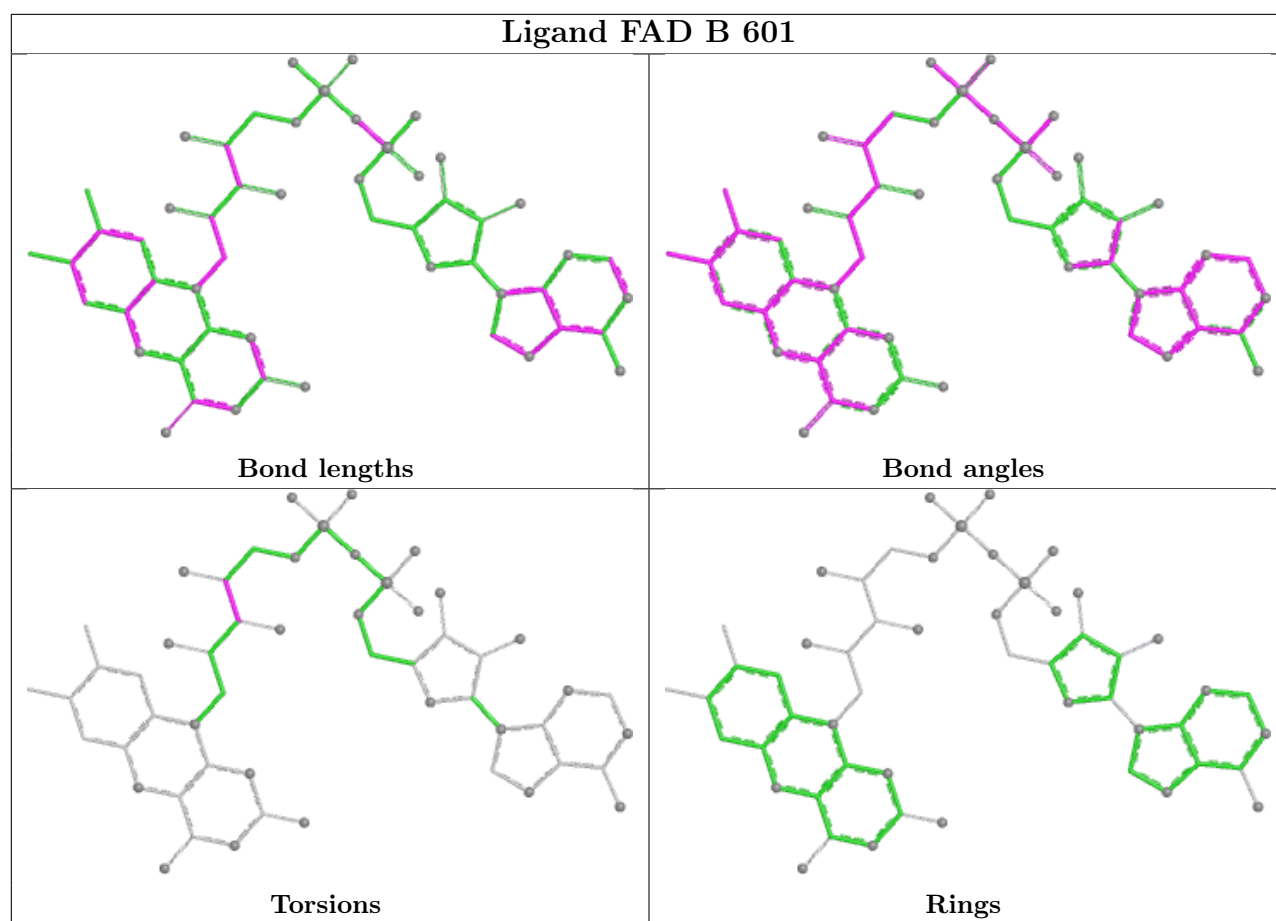
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	3	0
2	B	601	FAD	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	540/580 (93%)	0.36	26 (4%) 35 38	15, 26, 47, 77	0
1	B	540/580 (93%)	0.43	39 (7%) 21 23	16, 26, 47, 72	0
All	All	1080/1160 (93%)	0.39	65 (6%) 27 29	15, 26, 47, 77	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	ALA	7.1
1	B	467	PRO	6.4
1	B	416	TYR	5.0
1	A	416	TYR	4.8
1	B	414	LEU	4.6
1	B	428	HIS	4.5
1	B	464	GLU	4.2
1	B	209	ALA	4.1
1	B	418	TRP	4.0
1	A	380	PRO	4.0
1	A	160	THR	3.7
1	A	395	LEU	3.7
1	A	334	TRP	3.6
1	A	415	SER	3.5
1	A	215	ALA	3.5
1	A	428	HIS	3.5
1	A	555	GLN	3.4
1	B	395	LEU	3.4
1	A	414	LEU	3.3
1	A	464	GLU	3.2
1	B	555	GLN	3.2
1	B	291	SER	3.0
1	B	429	PRO	3.0
1	B	407	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	417	ALA	3.0
1	B	160	THR	2.9
1	A	467	PRO	2.9
1	A	418	TRP	2.9
1	A	417	ALA	2.8
1	A	498	VAL	2.8
1	B	221	HIS	2.7
1	B	559	ALA	2.7
1	A	205	TYR	2.7
1	B	255	ASP	2.7
1	B	462	SER	2.7
1	B	381	GLU	2.7
1	B	466	ASP	2.6
1	A	465	ALA	2.5
1	B	338	THR	2.5
1	A	350	LYS	2.4
1	B	560	ASP	2.4
1	B	216	LYS	2.4
1	B	350	LYS	2.4
1	B	380	PRO	2.4
1	B	405	GLY	2.4
1	A	381	GLU	2.4
1	A	499	GLU	2.3
1	A	216	LYS	2.3
1	B	342	CYS	2.3
1	B	155	LEU	2.3
1	A	140	GLU	2.3
1	B	499	GLU	2.2
1	B	217	LEU	2.1
1	B	148	LYS	2.1
1	B	408	LYS	2.1
1	B	278	GLU	2.1
1	A	150	ALA	2.1
1	B	150	ALA	2.1
1	A	382	THR	2.1
1	B	353	MET	2.1
1	A	383	GLY	2.0
1	B	220	GLN	2.0
1	B	151	ASP	2.0
1	A	448	THR	2.0
1	B	279	ARG	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](#)

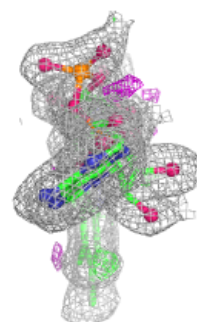
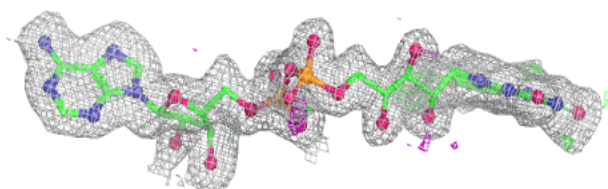
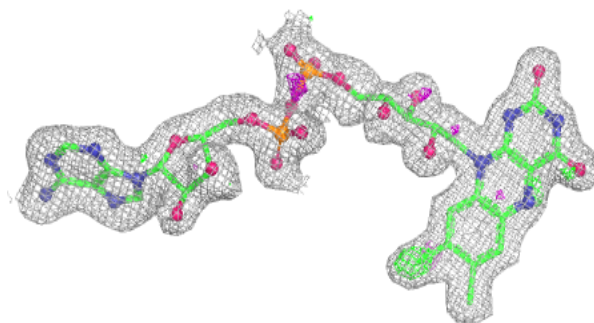
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	601	53/53	0.96	0.07	13,17,21,23	0
2	FAD	B	601	53/53	0.97	0.06	14,19,22,26	0

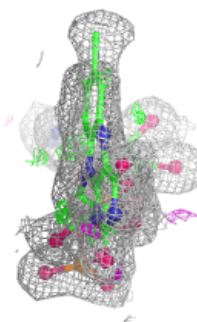
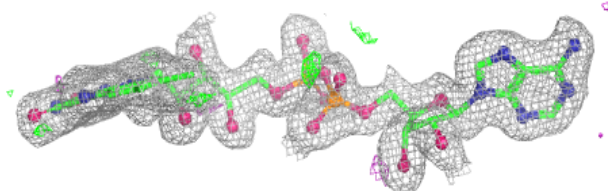
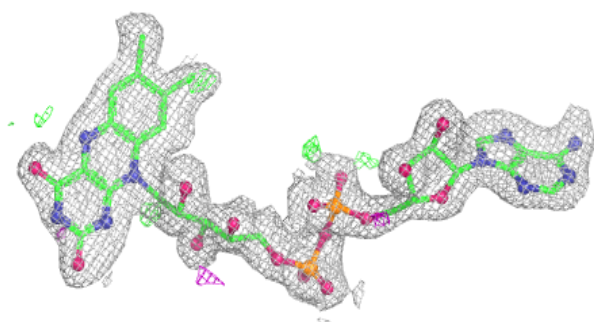
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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