



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:17 PM UTC

PDB ID : 2OAL / pdb_00002oal
Title : RebH with bound FAD
Authors : Blasiak, L.C.; Drennan, C.L.
Deposited on : 2006-12-16
Resolution : 2.10 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

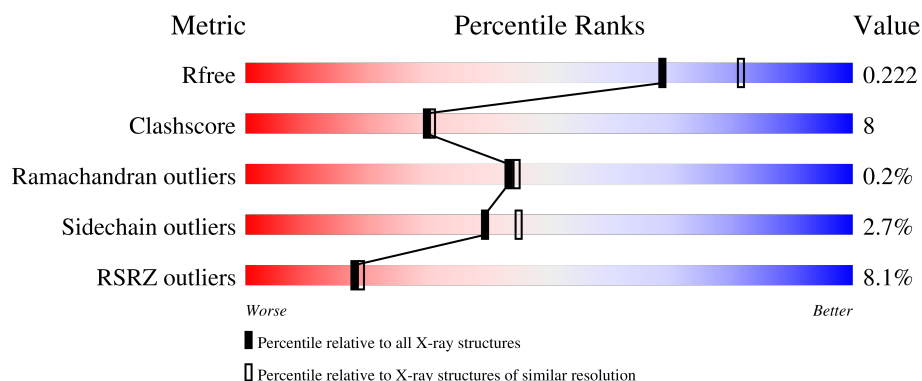
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	550	5% 78% 17% • •
1	B	550	11% 75% 20% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9136 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 Tryptophan halogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4224	2686	734	785	19			
1	B	528	Total	C	N	O	S	0	0	0
			4234	2691	737	787	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8KHZ8
A	-18	GLY	-	cloning artifact	UNP Q8KHZ8
A	-17	SER	-	cloning artifact	UNP Q8KHZ8
A	-16	SER	-	cloning artifact	UNP Q8KHZ8
A	-15	HIS	-	expression tag	UNP Q8KHZ8
A	-14	HIS	-	expression tag	UNP Q8KHZ8
A	-13	HIS	-	expression tag	UNP Q8KHZ8
A	-12	HIS	-	expression tag	UNP Q8KHZ8
A	-11	HIS	-	expression tag	UNP Q8KHZ8
A	-10	HIS	-	expression tag	UNP Q8KHZ8
A	-9	SER	-	cloning artifact	UNP Q8KHZ8
A	-8	SER	-	cloning artifact	UNP Q8KHZ8
A	-7	GLY	-	cloning artifact	UNP Q8KHZ8
A	-6	LEU	-	cloning artifact	UNP Q8KHZ8
A	-5	VAL	-	cloning artifact	UNP Q8KHZ8
A	-4	PRO	-	cloning artifact	UNP Q8KHZ8
A	-3	ARG	-	cloning artifact	UNP Q8KHZ8
A	-2	GLY	-	cloning artifact	UNP Q8KHZ8
A	-1	SER	-	cloning artifact	UNP Q8KHZ8
A	0	HIS	-	cloning artifact	UNP Q8KHZ8
B	-19	MET	-	initiating methionine	UNP Q8KHZ8
B	-18	GLY	-	cloning artifact	UNP Q8KHZ8
B	-17	SER	-	cloning artifact	UNP Q8KHZ8
B	-16	SER	-	cloning artifact	UNP Q8KHZ8
B	-15	HIS	-	expression tag	UNP Q8KHZ8

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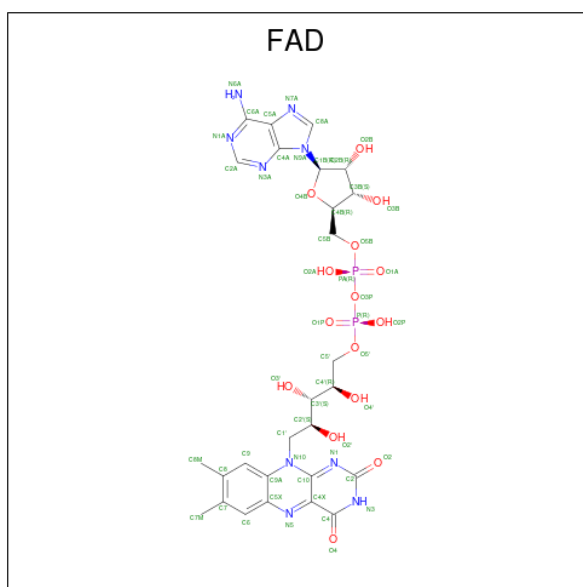
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q8KHZ8
B	-13	HIS	-	expression tag	UNP Q8KHZ8
B	-12	HIS	-	expression tag	UNP Q8KHZ8
B	-11	HIS	-	expression tag	UNP Q8KHZ8
B	-10	HIS	-	expression tag	UNP Q8KHZ8
B	-9	SER	-	cloning artifact	UNP Q8KHZ8
B	-8	SER	-	cloning artifact	UNP Q8KHZ8
B	-7	GLY	-	cloning artifact	UNP Q8KHZ8
B	-6	LEU	-	cloning artifact	UNP Q8KHZ8
B	-5	VAL	-	cloning artifact	UNP Q8KHZ8
B	-4	PRO	-	cloning artifact	UNP Q8KHZ8
B	-3	ARG	-	cloning artifact	UNP Q8KHZ8
B	-2	GLY	-	cloning artifact	UNP Q8KHZ8
B	-1	SER	-	cloning artifact	UNP Q8KHZ8
B	0	HIS	-	cloning artifact	UNP Q8KHZ8

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			52	27	9	14	2		

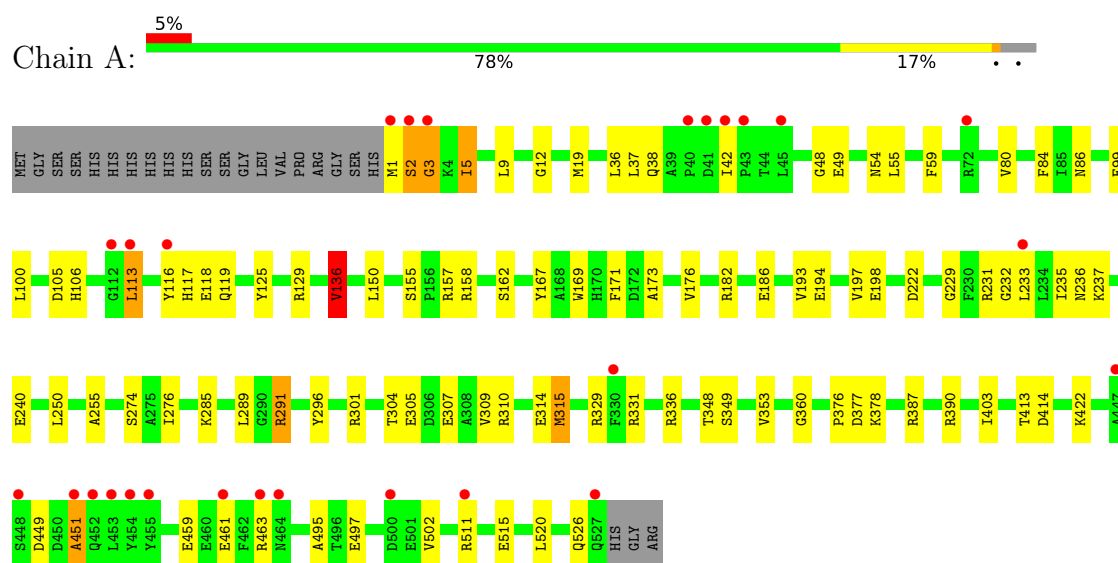
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	308	Total	O	0	0
			308	308		
4	B	264	Total	O	0	0
			264	264		

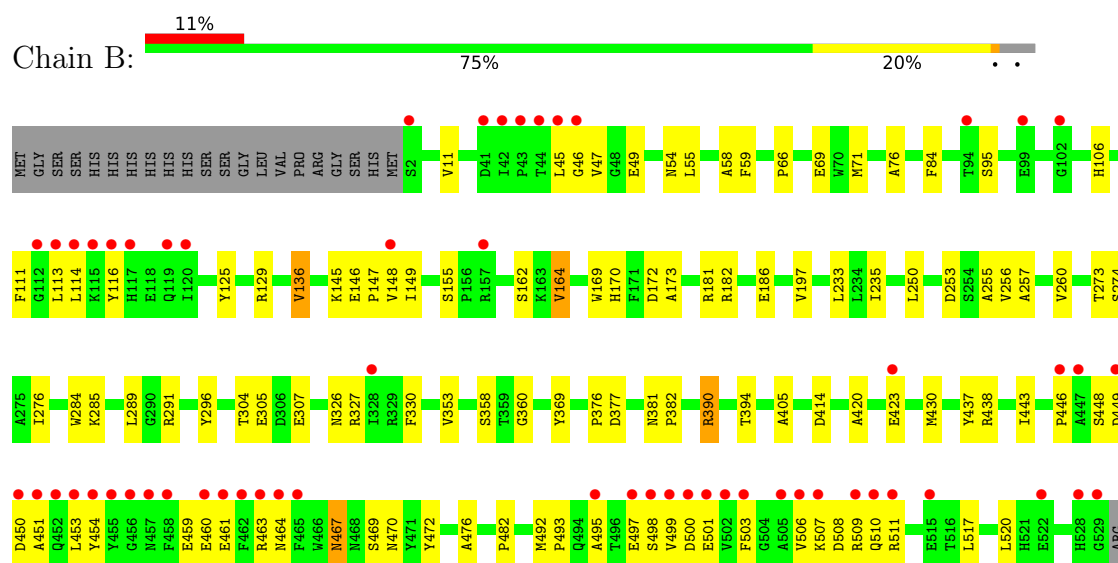
3 Residue-property plots

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: Tryptophan halogenase



• Molecule 1: Tryptophan halogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	114.72Å 114.72Å 230.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.90 – 2.10 35.90 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (35.90-2.10) 97.8 (35.90-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.81 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.222 0.197 , 0.222	Depositor DCC
R_{free} test set	4977 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9136	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, CL

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	0.43	1/4340 (0.0%)	0.91	14/5891 (0.2%)
1	B	0.37	0/4351	0.87	7/5905 (0.1%)
All	All	0.40	1/8691 (0.0%)	0.89	21/11796 (0.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	ALA	CA-CB	-5.93	1.44	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	SER	N-CA-C	10.04	132.19	110.80
1	A	3	GLY	N-CA-C	-8.91	97.27	112.51
1	A	48	GLY	N-CA-C	7.01	120.96	112.48
1	A	136	VAL	N-CA-C	-6.95	106.53	113.20
1	B	136	VAL	N-CA-C	-6.71	106.76	113.20
1	A	414	ASP	N-CA-C	6.62	120.62	112.54
1	B	111	PHE	N-CA-C	-6.58	105.25	113.28
1	B	377	ASP	N-CA-C	-6.46	99.58	109.65
1	A	235	ILE	N-CA-C	6.26	117.00	110.62
1	A	377	ASP	N-CA-C	-6.05	100.21	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	TRP	N-CA-C	5.85	118.59	109.52
1	A	5	ILE	N-CA-C	-5.58	102.33	109.30
1	A	331	ARG	N-CA-C	-5.55	98.16	107.99
1	A	349	SER	N-CA-C	-5.43	105.92	112.54
1	B	260	VAL	N-CA-C	5.34	113.96	107.61
1	B	235	ILE	N-CA-C	5.31	115.51	110.42
1	B	169	TRP	N-CA-C	5.27	117.68	109.52
1	B	414	ASP	N-CA-C	5.26	118.96	112.54
1	A	336	ARG	N-CA-C	-5.21	105.60	111.28
1	A	19	MET	N-CA-C	-5.16	105.74	111.36
1	A	502	VAL	N-CA-C	-5.03	104.69	111.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide

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	4224	0	4027	68	0
1	B	4234	0	4035	72	0
2	A	1	0	0	0	0
3	A	53	0	31	3	0
3	B	52	0	31	2	0
4	A	308	0	0	3	0
4	B	264	0	0	2	0
All	All	9136	0	8124	141	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 (141) 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:113:LEU:CD1	1:A:451:ALA:HB2	1.29	1.53
1:A:113:LEU:CD1	1:A:451:ALA:CB	2.24	1.15
1:A:113:LEU:HD22	1:A:113:LEU:H	1.11	1.13
1:A:113:LEU:H	1:A:113:LEU:CD2	1.66	1.06
1:A:113:LEU:HD11	1:A:451:ALA:HB2	1.12	1.06
1:A:113:LEU:HD12	1:A:451:ALA:HB2	1.08	1.05
1:A:113:LEU:HD12	1:A:451:ALA:CB	1.88	1.02
1:A:113:LEU:HD11	1:A:451:ALA:CB	1.92	0.97
1:A:113:LEU:HD22	1:A:113:LEU:N	1.82	0.93
1:A:49:GLU:HG3	1:A:173:ALA:HB2	1.52	0.92
1:B:113:LEU:HD21	1:B:451:ALA:HB2	1.50	0.92
1:B:45:LEU:H	1:B:326:ASN:HD21	1.25	0.84
1:B:49:GLU:HG3	1:B:173:ALA:HB2	1.62	0.82
1:B:467:ASN:HD22	1:B:469:SER:H	1.37	0.73
1:B:467:ASN:H	1:B:470:ASN:HD22	1.36	0.72
1:A:387:ARG:HH12	1:A:390:ARG:NH1	1.90	0.70
1:A:116:TYR:HD1	1:A:449:ASP:HB3	1.57	0.70
1:B:148:VAL:HG21	1:B:510:GLN:HB2	1.74	0.69
1:A:511:ARG:O	1:A:515:GLU:HG3	1.93	0.68
1:B:304:THR:OG1	1:B:307:GLU:HG3	1.94	0.68
1:B:405:ALA:HB2	1:B:430:MET:HE2	1.75	0.68
1:B:45:LEU:N	1:B:326:ASN:HD21	1.92	0.67
3:B:601:FAD:PA	3:B:601:FAD:P	2.93	0.66
1:B:148:VAL:CG2	1:B:510:GLN:HB2	2.25	0.66
1:A:12:GLY:HA2	3:A:600:FAD:H1B	1.78	0.66
1:B:113:LEU:HD21	1:B:451:ALA:CB	2.25	0.65
1:A:233:LEU:HD12	1:A:237:LYS:HD3	1.78	0.64
1:B:507:LYS:O	1:B:511:ARG:HG3	1.97	0.64
1:A:310:ARG:O	1:A:314:GLU:HG3	1.97	0.64
1:A:129:ARG:HD3	4:A:1178:HOH:O	1.96	0.63
1:B:498:SER:O	1:B:501:GLU:HG2	1.99	0.63
1:A:387:ARG:NH1	1:A:390:ARG:HD2	2.14	0.62
1:B:437:TYR:HB2	1:B:443:ILE:HD11	1.79	0.62
1:B:113:LEU:CD2	1:B:451:ALA:HB2	2.26	0.61
1:B:467:ASN:H	1:B:470:ASN:ND2	1.98	0.61
1:A:113:LEU:HD12	1:A:451:ALA:CA	2.31	0.60
1:A:197:VAL:HB	1:A:233:LEU:HD21	1.83	0.60
1:A:459:GLU:O	1:A:463:ARG:HD3	2.00	0.60
1:A:49:GLU:CG	1:A:173:ALA:HB2	2.29	0.60
1:B:450:ASP:OD1	1:B:453:LEU:HG	2.02	0.59
1:A:80:VAL:HB	1:A:150:LEU:HD21	1.83	0.59
1:B:503:PHE:O	1:B:506:VAL:HG22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:GLU:O	1:B:463:ARG:HG3	2.03	0.58
1:B:369:TYR:OH	1:B:459:GLU:HG2	2.03	0.58
1:B:164:VAL:HG11	1:B:517:LEU:HD21	1.87	0.56
1:A:158:ARG:HD2	1:A:162:SER:OG	2.06	0.56
1:B:467:ASN:HD22	1:B:469:SER:N	2.03	0.56
1:B:467:ASN:HD21	1:B:469:SER:HB2	1.71	0.56
1:A:413:THR:HG22	1:A:422:LYS:HE3	1.88	0.56
1:B:71:MET:HB2	1:B:76:ALA:HB3	1.88	0.55
1:A:5:ILE:HG23	1:A:222:ASP:HB2	1.87	0.55
1:A:182:ARG:O	1:A:186:GLU:HB2	2.06	0.54
1:B:274:SER:HB2	1:B:285:LYS:HB3	1.89	0.54
1:A:125:TYR:O	1:A:129:ARG:HG3	2.08	0.54
1:A:38:GLN:O	1:A:194:GLU:HA	2.09	0.53
1:B:467:ASN:ND2	1:B:469:SER:H	2.05	0.53
1:A:54:ASN:HD22	1:A:461:GLU:CD	2.17	0.53
1:A:305:GLU:O	1:A:309:VAL:HG23	2.09	0.52
1:B:467:ASN:N	1:B:470:ASN:HD22	2.05	0.52
1:A:37:LEU:HD23	1:A:193:VAL:HB	1.92	0.51
1:A:116:TYR:CD1	1:A:449:ASP:HB3	2.42	0.51
1:A:231:ARG:HG2	4:A:1306:HOH:O	2.11	0.51
1:B:420:ALA:HA	1:B:423:GLU:OE2	2.11	0.50
1:A:387:ARG:HH12	1:A:390:ARG:HD2	1.76	0.50
1:B:509:ARG:HD2	4:B:789:HOH:O	2.11	0.50
1:A:250:LEU:HD13	1:A:353:VAL:HG23	1.93	0.50
1:A:459:GLU:HG3	1:A:463:ARG:HH11	1.78	0.49
1:B:182:ARG:O	1:B:186:GLU:HB2	2.12	0.49
1:B:305:GLU:OE2	1:B:327:ARG:HD3	2.13	0.49
1:A:387:ARG:HH12	1:A:390:ARG:HH11	1.59	0.49
1:B:256:VAL:O	1:B:256:VAL:HG23	2.12	0.49
1:B:66:PRO:HG2	1:B:69:GLU:HB2	1.95	0.49
1:B:492:MET:HB3	1:B:495:ALA:HB3	1.94	0.49
1:A:84:PHE:O	1:A:106:HIS:HA	2.13	0.48
1:B:113:LEU:HD11	1:B:451:ALA:HB2	1.95	0.48
1:B:508:ASP:OD1	1:B:511:ARG:NH2	2.46	0.48
1:B:113:LEU:HD11	1:B:451:ALA:CB	2.45	0.47
1:B:155:SER:HB2	1:B:520:LEU:HA	1.96	0.47
1:B:116:TYR:CD2	1:B:449:ASP:HB3	2.49	0.47
1:A:12:GLY:HA2	3:A:600:FAD:C1B	2.44	0.47
1:A:3:GLY:O	1:A:378:LYS:HG3	2.15	0.47
1:B:145:LYS:HD3	1:B:509:ARG:HG2	1.96	0.47
1:A:353:VAL:HG21	1:A:403:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:VAL:HG11	1:B:233:LEU:HD21	1.96	0.46
1:B:55:LEU:O	1:B:59:PHE:HB3	2.15	0.46
1:A:233:LEU:O	1:A:237:LYS:HB3	2.15	0.46
1:A:54:ASN:ND2	1:A:461:GLU:OE1	2.41	0.46
1:A:117:HIS:HB3	1:A:125:TYR:CE2	2.51	0.46
1:A:229:GLY:HA2	1:A:348:THR:OG1	2.16	0.46
1:B:438:ARG:HA	1:B:482:PRO:HA	1.98	0.46
1:A:171:PHE:CE1	1:A:176:VAL:HG21	2.51	0.45
1:B:467:ASN:HD22	1:B:467:ASN:C	2.25	0.45
1:A:9:LEU:HD11	1:A:37:LEU:HG	1.98	0.45
1:B:113:LEU:HD21	1:B:451:ALA:CA	2.46	0.45
1:B:360:GLY:HA3	3:B:601:FAD:N1	2.32	0.44
1:B:289:LEU:HD12	1:B:289:LEU:N	2.33	0.44
1:A:360:GLY:HA3	3:A:600:FAD:H1'2	1.99	0.44
1:B:95:SER:HA	1:B:276:ILE:HD13	1.99	0.44
1:A:237:LYS:HD3	4:A:1213:HOH:O	2.18	0.44
1:B:170:HIS:NE2	1:B:273:THR:OG1	2.44	0.44
1:B:472:TYR:O	1:B:476:ALA:HB3	2.18	0.44
1:B:255:ALA:HA	1:B:296:TYR:O	2.18	0.43
1:A:157:ARG:NH1	1:A:167:TYR:OH	2.51	0.43
1:A:276:ILE:HG21	1:A:315:MET:HE1	1.98	0.43
1:B:47:VAL:HG11	1:B:257:ALA:CB	2.48	0.43
1:B:54:ASN:HB3	1:B:461:GLU:OE1	2.19	0.43
1:B:250:LEU:CD1	1:B:353:VAL:HG23	2.48	0.43
1:B:11:VAL:HG11	1:B:233:LEU:HD23	2.00	0.43
1:B:253:ASP:HA	1:B:330:PHE:CE1	2.54	0.43
1:A:113:LEU:H	1:A:113:LEU:HD23	1.70	0.43
1:B:113:LEU:CG	1:B:451:ALA:HB2	2.48	0.43
1:A:289:LEU:O	1:A:291:ARG:HD2	2.19	0.43
1:A:304:THR:OG1	1:A:307:GLU:HG3	2.19	0.42
1:A:86:ASN:HA	1:A:105:ASP:OD2	2.20	0.42
1:A:387:ARG:HH12	1:A:390:ARG:CZ	2.32	0.42
1:A:459:GLU:HG3	1:A:463:ARG:NH1	2.33	0.42
1:B:46:GLY:HA3	1:B:172:ASP:OD2	2.19	0.42
1:A:117:HIS:HE1	1:A:495:ALA:O	2.02	0.42
1:A:274:SER:HB2	1:A:285:LYS:HB3	2.00	0.42
1:A:255:ALA:HA	1:A:296:TYR:O	2.19	0.42
1:A:236:ASN:O	1:A:240:GLU:HA	2.19	0.42
1:B:136:VAL:HG12	1:B:136:VAL:O	2.20	0.42
1:A:231:ARG:O	1:A:232:GLY:C	2.61	0.42
1:A:36:LEU:C	1:A:36:LEU:HD23	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:O	1:A:136:VAL:HG13	2.20	0.42
1:A:155:SER:HB2	1:A:520:LEU:HA	2.01	0.42
1:B:181:ARG:HG2	1:B:181:ARG:HH11	1.85	0.42
1:B:250:LEU:HD13	1:B:353:VAL:HG23	2.02	0.41
1:B:148:VAL:HG23	1:B:149:ILE:N	2.35	0.41
1:B:493:PRO:O	1:B:497:GLU:HB2	2.20	0.41
1:A:55:LEU:O	1:A:59:PHE:HB3	2.20	0.41
1:B:84:PHE:O	1:B:106:HIS:HA	2.20	0.41
1:B:125:TYR:CG	1:B:499:VAL:HG21	2.55	0.41
1:B:162:SER:HA	4:B:675:HOH:O	2.20	0.41
1:B:446:PRO:HB2	1:B:448:SER:O	2.21	0.41
1:B:54:ASN:O	1:B:58:ALA:HB3	2.20	0.41
1:B:284:TRP:CD1	1:B:284:TRP:C	3.00	0.40
1:B:390:ARG:O	1:B:394:THR:HG23	2.21	0.40
1:A:118:GLU:O	1:A:119:GLN:HB2	2.21	0.40
1:B:146:GLU:HB2	1:B:147:PRO:HD3	2.04	0.40
1:B:381:ASN:HA	1:B:382:PRO:HD3	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	525/550 (96%)	511 (97%)	13 (2%)	1 (0%)	43	44
1	B	526/550 (96%)	504 (96%)	21 (4%)	1 (0%)	43	44
All	All	1051/1100 (96%)	1015 (97%)	34 (3%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER

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Mol	Chain	Res	Type
1	B	454	TYR

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	441/463 (95%)	428 (97%)	13 (3%)	37	42
1	B	443/463 (96%)	432 (98%)	11 (2%)	42	48
All	All	884/926 (96%)	860 (97%)	24 (3%)	39	45

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	99	GLU
1	A	100	LEU
1	A	113	LEU
1	A	136	VAL
1	A	198	GLU
1	A	291	ARG
1	A	301	ARG
1	A	315	MET
1	A	329	ARG
1	A	376	PRO
1	A	497	GLU
1	A	526	GLN
1	B	114	LEU
1	B	129	ARG
1	B	164	VAL
1	B	291	ARG
1	B	358	SER
1	B	376	PRO
1	B	390	ARG
1	B	460	GLU
1	B	464	ASN

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Mol	Chain	Res	Type
1	B	467	ASN
1	B	500	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	205	ASN
1	A	207	ASN
1	A	267	ASN
1	A	494	GLN
1	A	510	GLN
1	A	521	HIS
1	A	526	GLN
1	B	38	GLN
1	B	205	ASN
1	B	207	ASN
1	B	326	ASN
1	B	457	ASN
1	B	467	ASN
1	B	470	ASN
1	B	494	GLN
1	B	510	GLN
1	B	527	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	B	601	-	50,56,58	1.81	11 (22%)	71,82,89	1.70	14 (19%)
3	FAD	A	600	-	58,58,58	1.88	15 (25%)	85,89,89	1.67	13 (15%)

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	FAD	B	601	-	-	4/22/42/50	0/6/6/6
3	FAD	A	600	-	-	9/34/50/50	0/6/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	FAD	C4X-N5	5.44	1.42	1.30
3	A	600	FAD	C4X-N5	5.34	1.42	1.30
3	A	600	FAD	C10-N1	4.51	1.42	1.33
3	B	601	FAD	C10-N1	4.48	1.42	1.33
3	A	600	FAD	P-O3P	4.12	1.63	1.59
3	A	600	FAD	C1'-C2'	3.88	1.58	1.52
3	B	601	FAD	C2A-N3A	3.87	1.40	1.33
3	A	600	FAD	C2A-N1A	3.59	1.40	1.33
3	A	600	FAD	C2A-N3A	3.48	1.40	1.33
3	A	600	FAD	C8A-N7A	3.48	1.38	1.31
3	B	601	FAD	C2A-N1A	3.47	1.40	1.33
3	B	601	FAD	C8A-N7A	3.46	1.38	1.31
3	B	601	FAD	C1'-C2'	3.12	1.57	1.52
3	A	600	FAD	PA-O3P	3.09	1.62	1.59
3	A	600	FAD	C5'-C4'	2.90	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	FAD	C10-N10	2.86	1.43	1.37
3	A	600	FAD	C9-C9A	2.73	1.44	1.39
3	B	601	FAD	C10-N10	2.70	1.43	1.37
3	B	601	FAD	C9-C9A	2.62	1.43	1.39
3	A	600	FAD	C1'-N10	2.22	1.53	1.47
3	B	601	FAD	C6-C7	2.19	1.42	1.39
3	B	601	FAD	C4A-N3A	2.17	1.38	1.34
3	A	600	FAD	C4A-N3A	2.08	1.38	1.34
3	A	600	FAD	C9-C8	2.07	1.42	1.39
3	B	601	FAD	C9-C8	2.05	1.42	1.39
3	A	600	FAD	C9A-N10	2.03	1.44	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	FAD	N3A-C2A-N1A	-6.10	119.35	128.58
3	B	601	FAD	N3A-C2A-N1A	-5.92	119.62	128.58
3	A	600	FAD	N9A-C8A-N7A	-5.41	106.26	113.94
3	B	601	FAD	N9A-C8A-N7A	-5.26	106.47	113.94
3	A	600	FAD	C4A-N9A-C8A	3.93	109.86	105.74
3	B	601	FAD	C5A-N7A-C8A	3.64	109.18	103.45
3	B	601	FAD	C4A-N9A-C8A	3.64	109.56	105.74
3	A	600	FAD	O5'-C5'-C4'	3.63	119.06	109.36
3	A	600	FAD	C5A-N7A-C8A	3.43	108.84	103.45
3	A	600	FAD	C4A-N9A-C1B	-3.26	119.00	126.63
3	B	601	FAD	C5A-C4A-N3A	-3.19	122.33	126.72
3	B	601	FAD	C2A-N3A-C4A	2.96	119.05	111.83
3	A	600	FAD	C2A-N3A-C4A	2.88	118.87	111.83
3	A	600	FAD	O4'-C4'-C3'	2.82	115.85	109.25
3	B	601	FAD	O4'-C4'-C3'	2.80	115.80	109.25
3	A	600	FAD	C5A-C4A-N3A	-2.79	122.88	126.72
3	B	601	FAD	C4A-N9A-C1B	-2.70	120.33	126.63
3	B	601	FAD	C10-C4X-N5	-2.65	119.41	124.81
3	A	600	FAD	C10-C4X-N5	-2.62	119.46	124.81
3	B	601	FAD	N3A-C4A-N9A	2.29	131.06	127.17
3	B	601	FAD	C9A-C5X-N5	-2.21	120.11	122.45
3	A	600	FAD	C9A-C5X-N5	-2.19	120.13	122.45
3	A	600	FAD	C4X-C10-N10	2.11	119.50	116.48
3	B	601	FAD	C4A-C5A-N7A	-2.09	108.19	110.58
3	A	600	FAD	C5X-N5-C4X	2.08	121.45	118.09
3	B	601	FAD	C4X-C10-N10	2.03	119.38	116.48
3	B	601	FAD	C5X-N5-C4X	2.02	121.36	118.09

There are no chirality outliers.

All (13) torsion outliers are listed below:

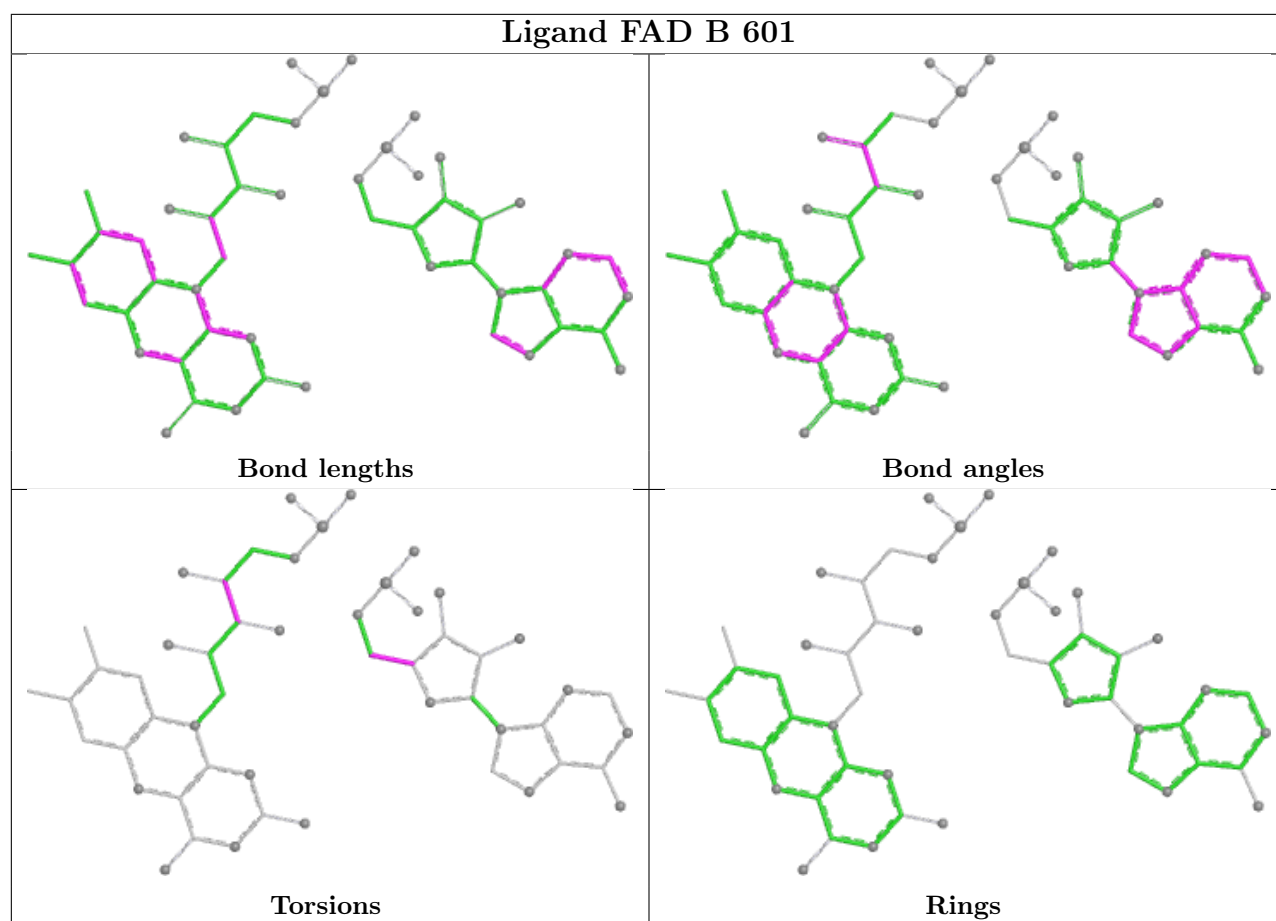
Mol	Chain	Res	Type	Atoms
3	A	600	FAD	C5B-O5B-PA-O1A
3	A	600	FAD	C5B-O5B-PA-O2A
3	A	600	FAD	C5B-O5B-PA-O3P
3	A	600	FAD	O3'-C3'-C4'-O4'
3	A	600	FAD	C2'-C3'-C4'-O4'
3	A	600	FAD	O3'-C3'-C4'-C5'
3	A	600	FAD	O4B-C4B-C5B-O5B
3	B	601	FAD	O3'-C3'-C4'-O4'
3	B	601	FAD	C2'-C3'-C4'-O4'
3	A	600	FAD	C3B-C4B-C5B-O5B
3	A	600	FAD	C2'-C3'-C4'-C5'
3	B	601	FAD	O3'-C3'-C4'-C5'
3	B	601	FAD	O4B-C4B-C5B-O5B

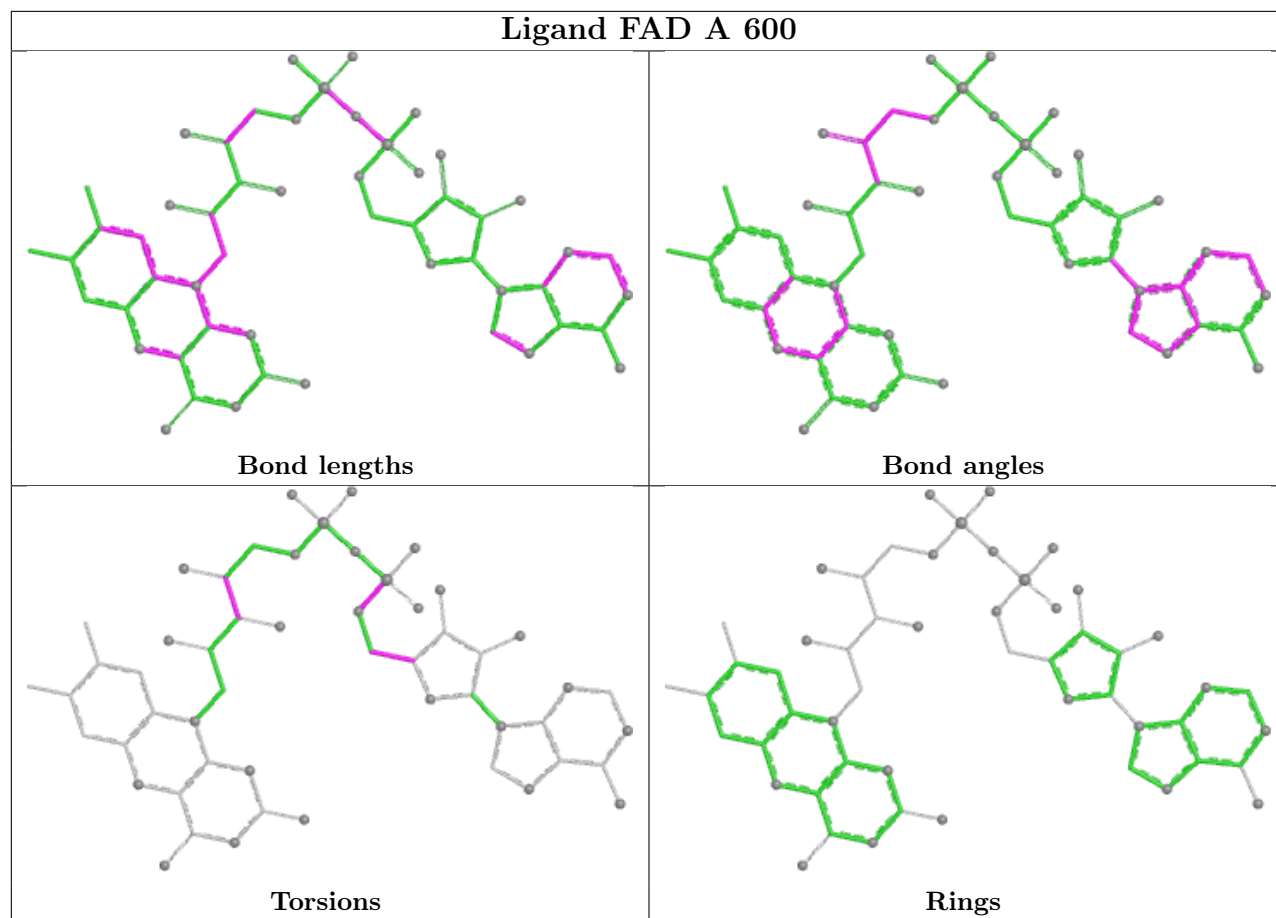
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	FAD	2	0
3	A	600	FAD	3	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	527/550 (95%)	0.17	27 (5%) 33 35	19, 33, 55, 74	0
1	B	528/550 (96%)	0.46	58 (10%) 10 11	20, 37, 66, 83	0
All	All	1055/1100 (95%)	0.32	85 (8%) 18 19	19, 35, 62, 83	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	451	ALA	6.9
1	B	453	LEU	5.7
1	A	453	LEU	5.5
1	A	113	LEU	5.0
1	B	113	LEU	5.0
1	A	454	TYR	4.9
1	B	456	GLY	4.3
1	B	42	ILE	4.2
1	B	112	GLY	4.0
1	B	45	LEU	4.0
1	A	452	GLN	4.0
1	A	451	ALA	3.8
1	B	454	TYR	3.7
1	B	447	ALA	3.7
1	B	529	GLY	3.7
1	B	116	TYR	3.7
1	A	42	ILE	3.5
1	B	464	ASN	3.5
1	A	112	GLY	3.4
1	A	2	SER	3.4
1	B	503	PHE	3.4
1	A	40	PRO	3.4
1	B	499	VAL	3.3
1	B	452	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	455	TYR	3.3
1	B	505	ALA	3.2
1	A	455	TYR	3.2
1	B	501	GLU	3.1
1	B	460	GLU	3.1
1	B	528	HIS	3.0
1	B	114	LEU	3.0
1	B	461	GLU	3.0
1	A	447	ALA	2.9
1	A	41	ASP	2.9
1	B	44	THR	2.9
1	B	119	GLN	2.9
1	A	330	PHE	2.8
1	B	46	GLY	2.8
1	B	423	GLU	2.8
1	A	1	MET	2.7
1	B	2	SER	2.7
1	A	233	LEU	2.6
1	B	446	PRO	2.6
1	B	465	PHE	2.6
1	A	463	ARG	2.6
1	B	497	GLU	2.5
1	B	41	ASP	2.5
1	A	527	GLN	2.5
1	B	120	ILE	2.5
1	B	450	ASP	2.4
1	B	498	SER	2.4
1	B	502	VAL	2.4
1	B	102	GLY	2.4
1	B	99	GLU	2.3
1	A	72	ARG	2.3
1	B	157	ARG	2.3
1	B	458	PHE	2.3
1	A	116	TYR	2.3
1	B	463	ARG	2.3
1	A	448	SER	2.3
1	A	461	GLU	2.3
1	B	506	VAL	2.3
1	B	511	ARG	2.3
1	B	500	ASP	2.3
1	B	462	PHE	2.2
1	B	148	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	509	ARG	2.2
1	B	328	ILE	2.2
1	A	45	LEU	2.2
1	B	515	GLU	2.1
1	B	94	THR	2.1
1	B	510	GLN	2.1
1	A	3	GLY	2.1
1	B	117	HIS	2.1
1	A	464	ASN	2.1
1	B	457	ASN	2.1
1	B	522	GLU	2.1
1	A	500	ASP	2.1
1	B	449	ASP	2.1
1	B	507	LYS	2.1
1	A	43	PRO	2.1
1	A	511	ARG	2.1
1	B	43	PRO	2.1
1	B	495	ALA	2.1
1	B	115	LYS	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](#)

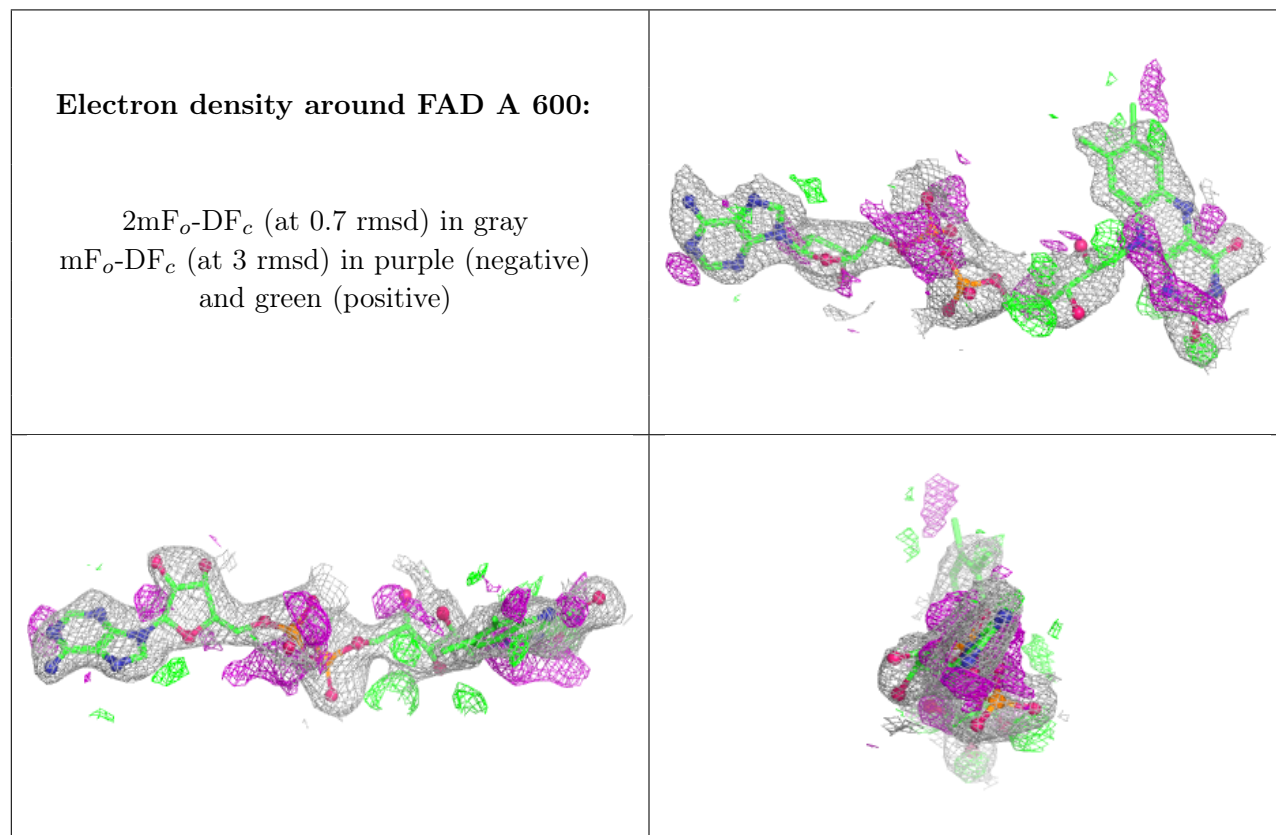
There are no oligosaccharides in this entry.

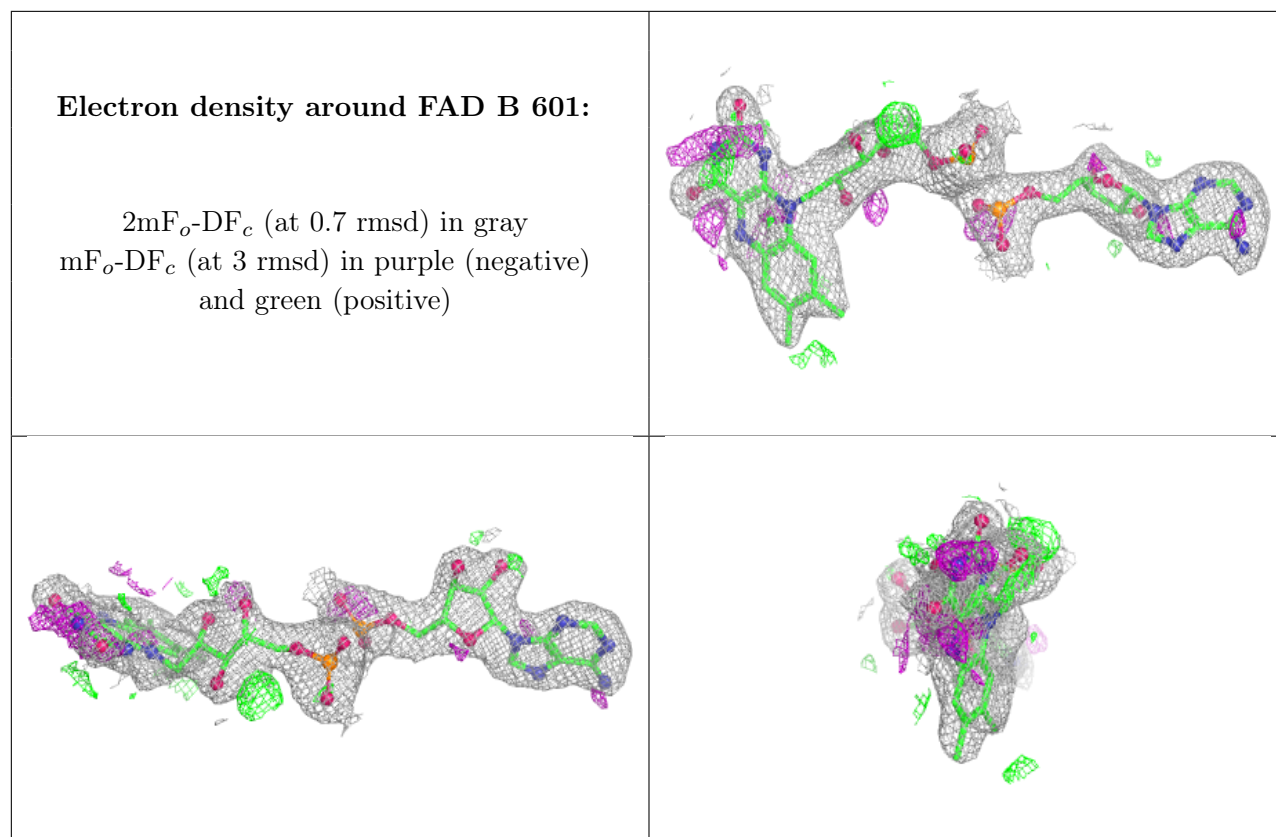
6.4 Ligands [i](#)

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	FAD	A	600	53/53	0.79	0.18	57,68,75,77	0
3	FAD	B	601	52/53	0.89	0.13	42,54,62,63	0
2	CL	A	1000	1/1	0.95	0.16	71,71,71,71	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.