



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:05 PM UTC

PDB ID : 2JB3 / pdb_00002jb3
Title : The structure of L-amino acid oxidase from *Rhodococcus opacus* in complex with o-aminobenzoate
Authors : Faust, A.; Niefind, K.; hummel, W.; Schomburg, D.
Deposited on : 2006-12-01
Resolution : 1.85 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

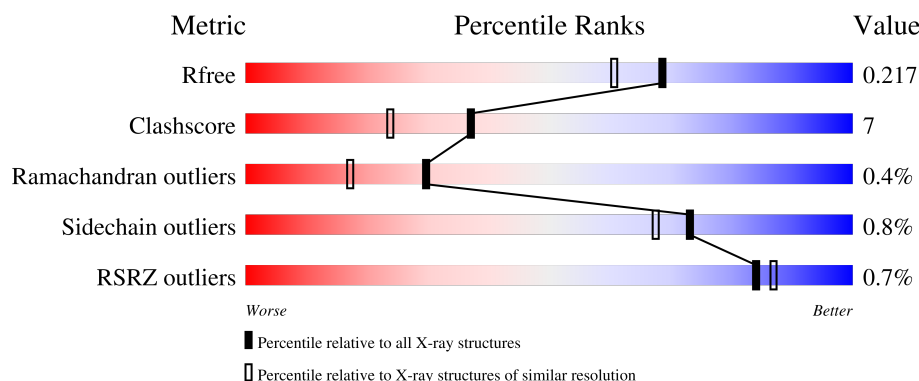
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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.

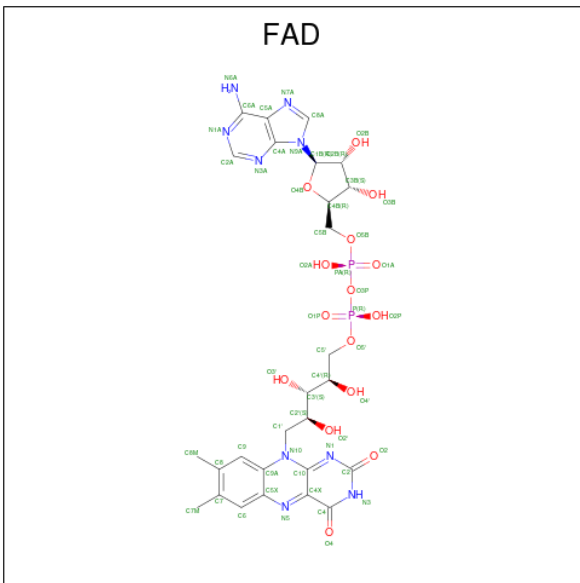
Mol	Chain	Length	Quality of chain
1	A	489	
1	B	489	

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.

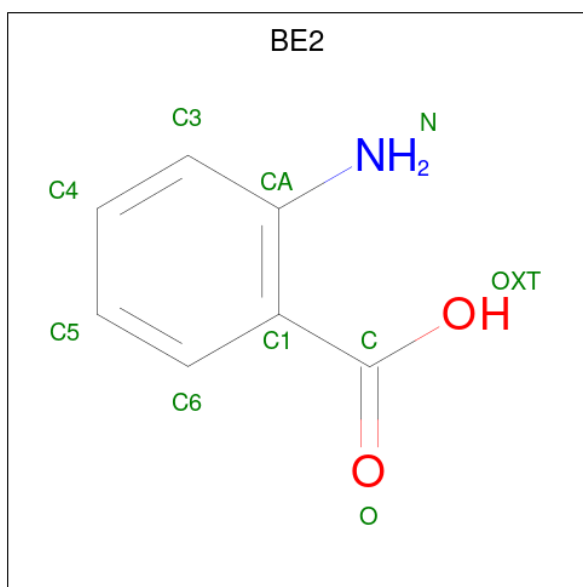
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total 3707	C 2311	N 649	O 735	S 12	0	5	1
1	B	477	Total 3693	C 2308	N 645	O 728	S 12	0	0	0

- 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 2-AMINOBENZOIC ACID (CCD ID: BE2) (formula: $C_7H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	7	1	2		
3	B	1	Total	C	N	O	0	0
			10	7	1	2		

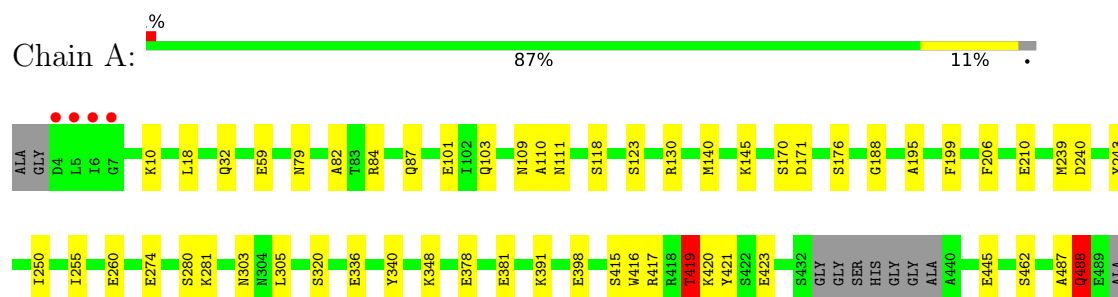
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	481	Total	O	0	0
			481	481		
4	B	504	Total	O	0	0
			504	504		

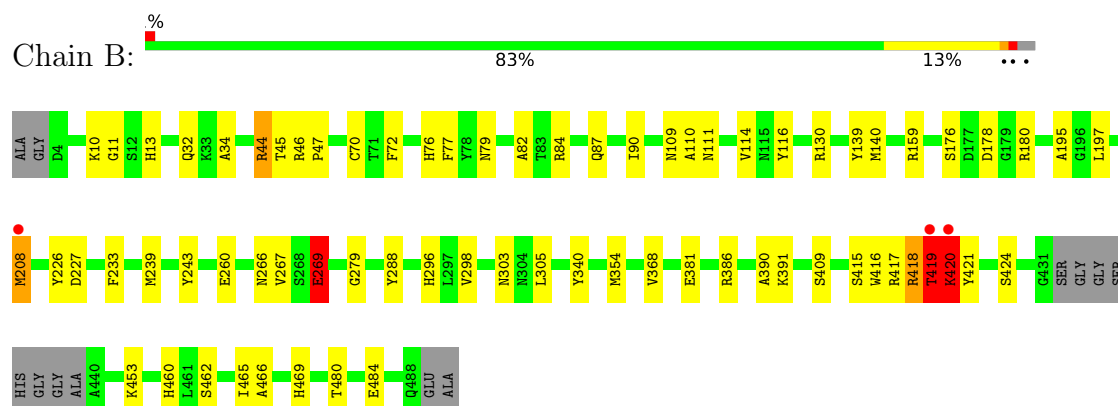
3 Residue-property plots

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: L-AMINO ACID OXIDASE



• Molecule 1: L-AMINO ACID OXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.65Å 109.68Å 134.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.77 – 1.85 19.77 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.77-1.85) 99.1 (19.77-1.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.151 , 0.214 0.156 , 0.217	Depositor DCC
R_{free} test set	4145 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8511	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, BE2

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	0.78	1/3811 (0.0%)	0.83	0/5146
1	B	0.80	1/3770 (0.0%)	0.88	4/5086 (0.1%)
All	All	0.79	2/7581 (0.0%)	0.86	4/10232 (0.0%)

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	17
1	B	0	20
All	All	0	37

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	488	GLN	C-N	-6.23	1.24	1.33
1	B	208	MET	CG-SD	5.20	1.93	1.80

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	THR	CB-CA-C	9.42	125.21	110.14
1	B	418	ARG	CA-C-N	-7.66	111.98	122.77
1	B	418	ARG	C-N-CA	-7.66	111.98	122.77
1	B	419	THR	N-CA-C	5.53	117.40	108.34

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	GLU	Sidechain
1	A	199	PHE	Sidechain
1	A	206	PHE	Sidechain
1	A	210	GLU	Mainchain
1	A	240	ASP	Sidechain
1	A	243	TYR	Sidechain
1	A	255	ILE	Mainchain
1	A	260	GLU	Sidechain
1	A	274	GLU	Sidechain
1	A	280	SER	Mainchain
1	A	336	GLU	Sidechain
1	A	378	GLU	Sidechain
1	A	391	LYS	Mainchain
1	A	419	THR	Mainchain
1	A	423	GLU	Sidechain
1	A	488	GLN	Mainchain
1	A	59	GLU	Sidechain
1	B	11	GLY	Mainchain
1	B	159	ARG	Sidechain
1	B	180	ARG	Sidechain
1	B	227	ASP	Sidechain
1	B	233	PHE	Sidechain
1	B	243	TYR	Sidechain
1	B	260	GLU	Sidechain
1	B	269	GLU	Mainchain
1	B	279	GLY	Mainchain
1	B	288	TYR	Sidechain
1	B	298	VAL	Mainchain
1	B	34	ALA	Mainchain
1	B	386	ARG	Sidechain
1	B	409	SER	Mainchain
1	B	417	ARG	Sidechain
1	B	418	ARG	Sidechain
1	B	419	THR	Mainchain
1	B	44	ARG	Sidechain
1	B	460	HIS	Mainchain
1	B	77	PHE	Sidechain

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	3707	0	3547	40	0
1	B	3693	0	3533	77	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	10	0	3	1	0
3	B	10	0	3	1	0
4	A	481	0	0	8	1
4	B	504	0	0	15	1
All	All	8511	0	7148	104	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (104) 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:420:LYS:HG3	4:B:2056:HOH:O	1.40	1.18
1:B:419:THR:HG23	1:B:420:LYS:CE	1.77	1.14
1:B:420:LYS:HG2	1:B:420:LYS:O	1.51	1.08
1:B:420:LYS:CG	4:B:2056:HOH:O	1.98	1.00
1:B:419:THR:C	1:B:420:LYS:HD3	1.86	1.00
1:B:420:LYS:HB3	4:B:2437:HOH:O	1.62	0.99
1:B:419:THR:CG2	1:B:420:LYS:HE2	1.94	0.98
1:B:419:THR:HG23	1:B:420:LYS:HE2	0.97	0.97
1:B:390:ALA:C	1:B:391:LYS:CA	2.39	0.94
1:B:420:LYS:CB	4:B:2056:HOH:O	2.18	0.89
1:B:419:THR:OG1	1:B:420:LYS:HD2	1.74	0.88
1:A:303:ASN:HD22	1:A:305:LEU:H	1.22	0.87
1:B:420:LYS:O	1:B:420:LYS:CG	2.19	0.87
1:B:419:THR:CB	1:B:420:LYS:HD3	2.04	0.87
1:B:45:THR:C	1:B:46:ARG:CA	2.50	0.84
1:B:420:LYS:HB2	4:B:2056:HOH:O	1.75	0.84
1:A:145:LYS:NZ	4:A:2168:HOH:O	2.10	0.83
1:B:419:THR:CA	1:B:420:LYS:HD3	2.08	0.83
1:B:419:THR:OG1	1:B:420:LYS:CD	2.27	0.82
1:B:90:ILE:H	1:B:469:HIS:HD2	1.24	0.81
1:A:87:GLN:HE22	1:B:109:ASN:HD21	1.28	0.81
1:A:79:ASN:HD21	1:A:239:MET:H	1.27	0.80
1:A:109:ASN:HD21	1:B:87:GLN:HE22	1.30	0.80
1:B:32:GLN:NE2	4:B:2021:HOH:O	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASN:HD21	1:B:239:MET:H	1.32	0.77
1:B:269:GLU:OE2	4:B:2297:HOH:O	2.02	0.77
1:B:44:ARG:NH2	1:B:420:LYS:HE3	2.02	0.75
1:A:87:GLN:HE21	1:B:340:TYR:H	1.31	0.74
1:A:171:ASP:OD2	4:A:2191:HOH:O	2.05	0.74
1:B:303:ASN:HD22	1:B:305:LEU:H	1.36	0.74
1:A:487:ALA:O	1:A:488:GLN:HB2	1.89	0.73
1:B:419:THR:CB	1:B:420:LYS:CD	2.67	0.73
1:A:140:MET:CE	1:B:140:MET:HE3	2.20	0.72
1:B:296:HIS:CD2	4:B:2334:HOH:O	2.44	0.71
4:A:2178:HOH:O	1:B:208:MET:HB3	1.91	0.69
1:A:87:GLN:NE2	1:B:340:TYR:H	1.91	0.68
1:A:170[B]:SER:OG	4:A:2190:HOH:O	2.10	0.68
1:B:419:THR:CG2	1:B:420:LYS:CE	2.63	0.68
1:B:296:HIS:HD2	4:B:2334:HOH:O	1.77	0.67
1:A:111:ASN:HD21	1:A:130:ARG:HH21	1.44	0.65
1:B:139:TYR:CE1	1:B:208:MET:HG2	2.31	0.64
1:A:416:TRP:HA	1:A:419:THR:HG23	1.80	0.64
1:B:82:ALA:HA	2:B:1489:FAD:C4X	2.29	0.62
1:A:82:ALA:HA	2:A:1489:FAD:C4X	2.29	0.62
1:B:415:SER:O	1:B:419:THR:HG22	2.00	0.62
1:A:103:GLN:NE2	4:A:2111:HOH:O	2.32	0.61
1:A:110:ALA:HB1	1:A:130:ARG:HB3	1.84	0.59
1:B:90:ILE:H	1:B:469:HIS:CD2	2.15	0.59
1:A:140:MET:HE1	1:B:140:MET:HE3	1.85	0.59
1:B:13:HIS:HD2	4:B:2316:HOH:O	1.85	0.59
1:B:46:ARG:NH1	4:B:2042:HOH:O	2.40	0.55
1:B:44:ARG:HH21	1:B:420:LYS:HE3	1.72	0.55
1:B:419:THR:OG1	1:B:420:LYS:HD3	1.99	0.55
1:A:111:ASN:ND2	1:A:130:ARG:HH21	2.06	0.54
1:A:281:LYS:NZ	4:A:2311:HOH:O	2.35	0.54
1:A:140:MET:HE2	1:B:140:MET:HE3	1.91	0.53
1:B:419:THR:C	1:B:420:LYS:CD	2.72	0.52
1:A:84:ARG:HH21	3:A:1490:BE2:C	2.23	0.52
1:B:76:HIS:HD2	4:B:2395:HOH:O	1.92	0.52
1:A:195:ALA:HA	1:B:462:SER:HA	1.92	0.51
1:A:415:SER:O	1:A:419:THR:HG22	2.09	0.51
1:B:47:PRO:C	4:B:2042:HOH:O	2.53	0.51
1:B:419:THR:HG23	1:B:420:LYS:CD	2.39	0.51
1:A:32:GLN:HB2	4:A:2010:HOH:O	2.12	0.50
1:B:44:ARG:NH2	1:B:420:LYS:HG2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HH21	1:B:420:LYS:CE	2.24	0.50
1:B:208:MET:HG3	4:B:2237:HOH:O	2.11	0.49
1:B:419:THR:CG2	1:B:420:LYS:CD	2.90	0.49
1:B:266:ASN:HD21	1:B:453:LYS:H	1.61	0.48
1:B:111:ASN:ND2	1:B:130:ARG:HE	2.11	0.47
1:B:84:ARG:HH21	3:B:1490:BE2:C	2.27	0.47
1:A:340:TYR:H	1:B:87:GLN:NE2	2.12	0.47
1:B:44:ARG:HH21	1:B:420:LYS:CG	2.28	0.47
1:A:320[A]:SER:OG	1:A:381:GLU:OE1	2.17	0.47
1:B:10:LYS:O	1:B:13:HIS:CE1	2.68	0.47
1:B:79:ASN:ND2	1:B:239:MET:H	2.08	0.47
1:A:79:ASN:ND2	1:A:239:MET:H	2.05	0.46
1:A:415:SER:O	1:A:419:THR:CG2	2.63	0.46
1:B:420:LYS:O	1:B:421:TYR:HB2	2.16	0.46
1:B:354:MET:HB2	1:B:368:VAL:HB	1.98	0.46
1:B:465:ILE:O	1:B:466:ALA:HB3	2.16	0.45
1:B:110:ALA:HB1	1:B:130:ARG:HB3	1.97	0.45
1:B:267:VAL:O	1:B:453:LYS:NZ	2.50	0.45
1:B:296:HIS:CD2	1:B:296:HIS:H	2.33	0.45
1:B:176:SER:OG	1:B:178:ASP:OD2	2.31	0.44
1:B:381:GLU:HG3	1:B:415:SER:OG	2.17	0.44
1:A:445:GLU:HG2	1:B:197:LEU:HD21	1.99	0.44
1:A:419:THR:HG21	4:A:2431:HOH:O	2.17	0.44
1:A:348:LYS:HE2	1:A:398:GLU:OE1	2.17	0.44
1:B:419:THR:HG21	4:B:2436:HOH:O	2.16	0.44
1:A:340:TYR:H	1:B:87:GLN:HE21	1.66	0.44
1:A:303:ASN:ND2	1:A:305:LEU:H	2.03	0.43
1:B:10:LYS:O	1:B:13:HIS:HE1	2.02	0.42
1:B:70:CYS:SG	1:B:72:PHE:CD2	3.11	0.42
1:A:18:LEU:HD12	1:A:18:LEU:N	2.34	0.42
1:A:32:GLN:HE22	1:A:250:ILE:HA	1.84	0.42
1:A:188:GLY:HA2	1:B:226:TYR:CE1	2.54	0.42
1:A:118:SER:O	1:A:123:SER:HB2	2.21	0.41
1:A:420:LYS:HG2	1:A:421:TYR:CD2	2.56	0.41
1:B:480:THR:O	1:B:484:GLU:HG3	2.20	0.41
1:A:462:SER:HA	1:B:195:ALA:HA	2.03	0.41
1:B:416:TRP:CZ3	1:B:420:LYS:NZ	2.85	0.41
1:B:114:VAL:HB	1:B:116:TYR:CE2	2.56	0.40
1:A:111:ASN:ND2	1:A:130:ARG:HE	2.20	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2297:HOH:O	4:B:2235:HOH:O[3_645]	2.16	0.04

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	480/489 (98%)	466 (97%)	12 (2%)	2 (0%)	30	17
1	B	469/489 (96%)	454 (97%)	13 (3%)	2 (0%)	30	17
All	All	949/978 (97%)	920 (97%)	25 (3%)	4 (0%)	30	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	GLN
1	B	420	LYS
1	A	176	SER
1	B	424	SER

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	392/390 (100%)	388 (99%)	4 (1%)	68	60
1	B	384/390 (98%)	382 (100%)	2 (0%)	81	77
All	All	776/780 (100%)	770 (99%)	6 (1%)	73	67

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	417	ARG
1	A	419	THR
1	A	488	GLN
1	B	269	GLU
1	B	420	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	76	HIS
1	A	79	ASN
1	A	87	GLN
1	A	89	HIS
1	A	103	GLN
1	A	108	GLN
1	A	111	ASN
1	A	150	GLN
1	A	303	ASN
1	A	481	HIS
1	B	13	HIS
1	B	76	HIS
1	B	79	ASN
1	B	87	GLN
1	B	103	GLN
1	B	108	GLN
1	B	111	ASN
1	B	125	GLN
1	B	266	ASN
1	B	296	HIS
1	B	303	ASN
1	B	345	ASN
1	B	428	ASN
1	B	463	ASN
1	B	468	GLN
1	B	469	HIS
1	B	488	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 ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	A	1489	-	58,58,58	1.14	4 (6%)	85,89,89	1.59	16 (18%)
2	FAD	B	1489	-	58,58,58	1.20	6 (10%)	85,89,89	1.59	13 (15%)
3	BE2	B	1490	-	10,10,10	1.80	1 (10%)	13,13,13	1.74	3 (23%)
3	BE2	A	1490	-	10,10,10	1.95	1 (10%)	13,13,13	1.66	2 (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
2	FAD	A	1489	-	-	1/34/50/50	0/6/6/6
2	FAD	B	1489	-	-	2/34/50/50	0/6/6/6
3	BE2	B	1490	-	-	4/4/4/4	0/1/1/1
3	BE2	A	1490	-	-	4/4/4/4	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1490	BE2	C1-CA	5.48	1.49	1.41
3	B	1490	BE2	C1-CA	5.15	1.49	1.41
2	B	1489	FAD	C4X-N5	4.45	1.40	1.30
2	A	1489	FAD	C4X-N5	4.02	1.39	1.30
2	B	1489	FAD	PA-O3P	3.06	1.62	1.59
2	A	1489	FAD	PA-O3P	2.98	1.62	1.59
2	B	1489	FAD	C10-N1	2.52	1.38	1.33
2	B	1489	FAD	P-O3P	2.44	1.62	1.59
2	B	1489	FAD	C8A-N7A	2.43	1.36	1.31
2	A	1489	FAD	C2A-N3A	2.40	1.38	1.33
2	A	1489	FAD	C2A-N1A	2.39	1.38	1.33
2	B	1489	FAD	O4'-C4'	-2.21	1.38	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1489	FAD	N3A-C2A-N1A	-6.22	119.17	128.58
2	A	1489	FAD	N3A-C2A-N1A	-5.02	120.99	128.58
2	A	1489	FAD	N9A-C8A-N7A	-4.74	107.21	113.94
2	B	1489	FAD	C5A-C4A-N3A	-4.12	121.04	126.72
2	A	1489	FAD	C5A-N7A-C8A	3.84	109.49	103.45
2	B	1489	FAD	N9A-C8A-N7A	-3.73	108.64	113.94
2	A	1489	FAD	C5A-C4A-N3A	-3.63	121.72	126.72
2	B	1489	FAD	C2A-N3A-C4A	3.46	120.29	111.83
2	B	1489	FAD	C9A-C5X-N5	-3.40	118.85	122.45
3	A	1490	BE2	CA-C1-C	-3.27	117.35	121.27
3	B	1490	BE2	C1-CA-N	-3.26	118.13	122.68
2	A	1489	FAD	C4A-N9A-C8A	3.15	109.05	105.74
2	A	1489	FAD	C4-N3-C2	-3.14	120.06	125.64
3	B	1490	BE2	CA-C1-C	-3.13	117.51	121.27
2	A	1489	FAD	C10-C4X-N5	-3.05	118.58	124.81
3	A	1490	BE2	C1-CA-N	-2.85	118.70	122.68
2	A	1489	FAD	C5'-C4'-C3'	-2.81	106.91	112.22
2	B	1489	FAD	C4-C4X-N5	2.69	121.93	118.21
2	A	1489	FAD	N3A-C4A-N9A	2.68	131.72	127.17
2	A	1489	FAD	C4A-C5A-N7A	-2.66	107.54	110.58
2	A	1489	FAD	C2A-N3A-C4A	2.66	118.32	111.83
2	B	1489	FAD	C5A-N7A-C8A	2.59	107.52	103.45
2	B	1489	FAD	C5X-C9A-N10	2.56	120.28	117.97
3	B	1490	BE2	C6-C1-CA	2.51	121.50	118.96
2	B	1489	FAD	O4B-C1B-N9A	2.51	112.92	108.09
2	B	1489	FAD	N3A-C4A-N9A	2.51	131.44	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1489	FAD	C4X-C10-N10	2.51	120.07	116.48
2	A	1489	FAD	C4-C4X-N5	2.51	121.67	118.21
2	B	1489	FAD	C10-C4X-N5	-2.51	119.69	124.81
2	A	1489	FAD	C4X-C4-N3	2.40	119.35	113.25
2	A	1489	FAD	O4B-C1B-N9A	2.38	112.66	108.09
2	A	1489	FAD	C6A-C5A-C4A	2.17	120.14	117.18
2	B	1489	FAD	C9A-C9-C8	2.12	123.48	119.22
2	B	1489	FAD	C4X-C4-N3	2.00	118.35	113.25

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1489	FAD	PA-O3P-P-O5'
2	B	1489	FAD	PA-O3P-P-O5'
3	A	1490	BE2	OXT-C-C1-CA
3	A	1490	BE2	O-C-C1-CA
3	B	1490	BE2	O-C-C1-CA
3	A	1490	BE2	O-C-C1-C6
3	B	1490	BE2	OXT-C-C1-CA
3	B	1490	BE2	O-C-C1-C6
3	B	1490	BE2	OXT-C-C1-C6
3	A	1490	BE2	OXT-C-C1-C6
2	B	1489	FAD	O4B-C4B-C5B-O5B

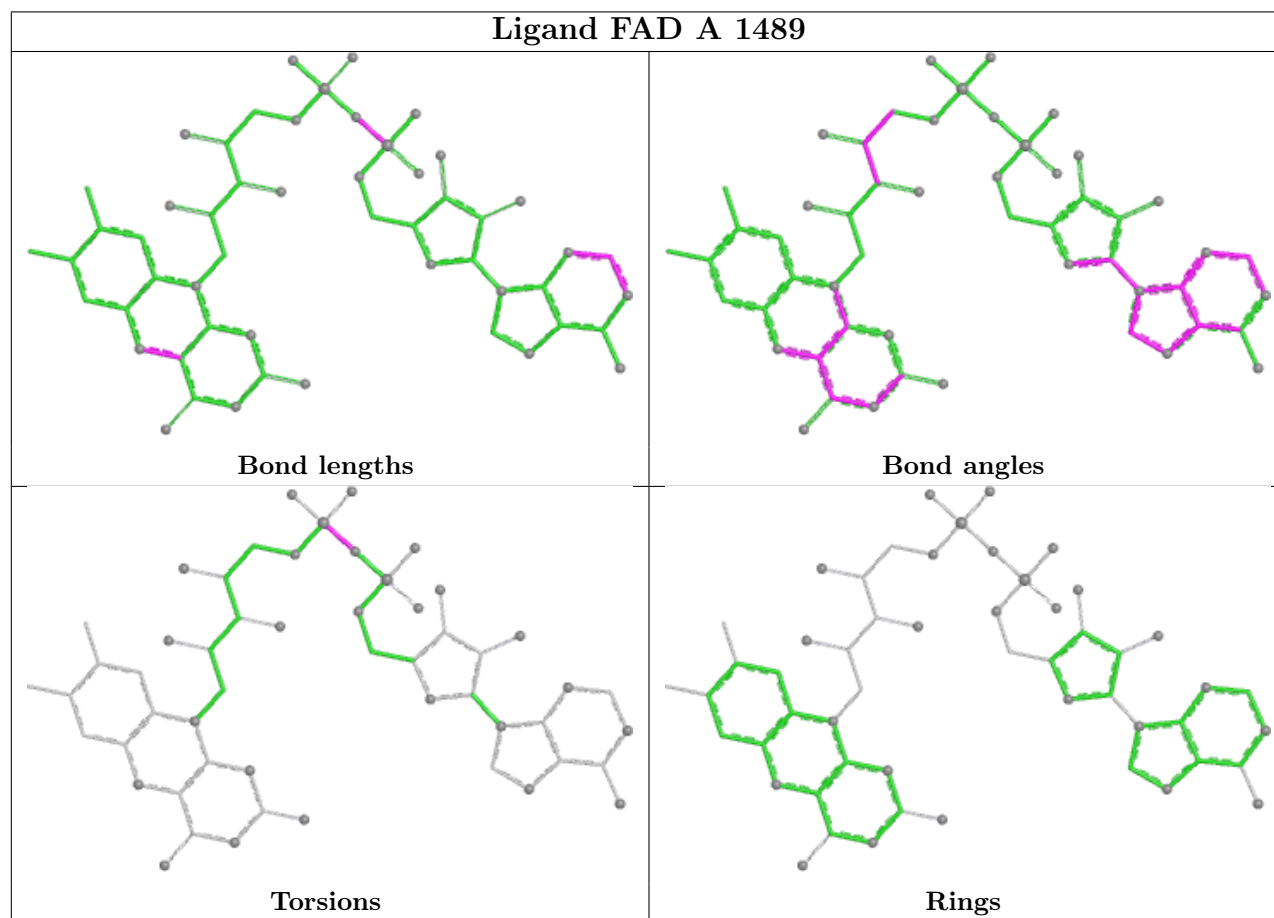
There are no ring outliers.

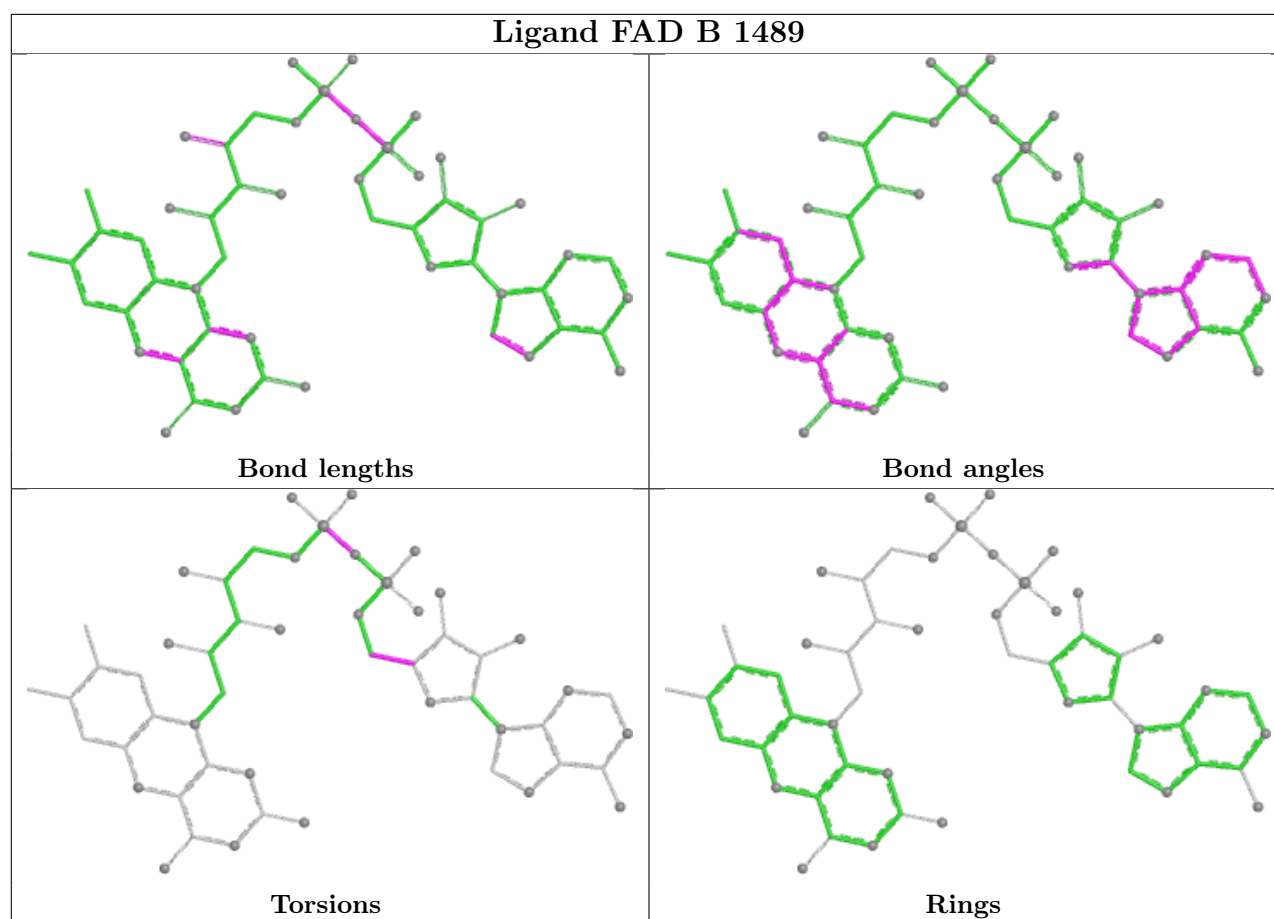
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1489	FAD	1	0
2	B	1489	FAD	1	0
3	B	1490	BE2	1	0
3	A	1490	BE2	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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	479/489 (97%)	-0.47	4 (0%) 82 86	10, 17, 28, 54	5 (1%)
1	B	477/489 (97%)	-0.47	3 (0%) 85 88	10, 17, 28, 38	0
All	All	956/978 (97%)	-0.47	7 (0%) 84 87	10, 17, 28, 54	5 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	420	LYS	5.4
1	B	419	THR	3.1
1	B	208	MET	3.0
1	A	5	LEU	3.0
1	A	7	GLY	2.6
1	A	6	ILE	2.2
1	A	4	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

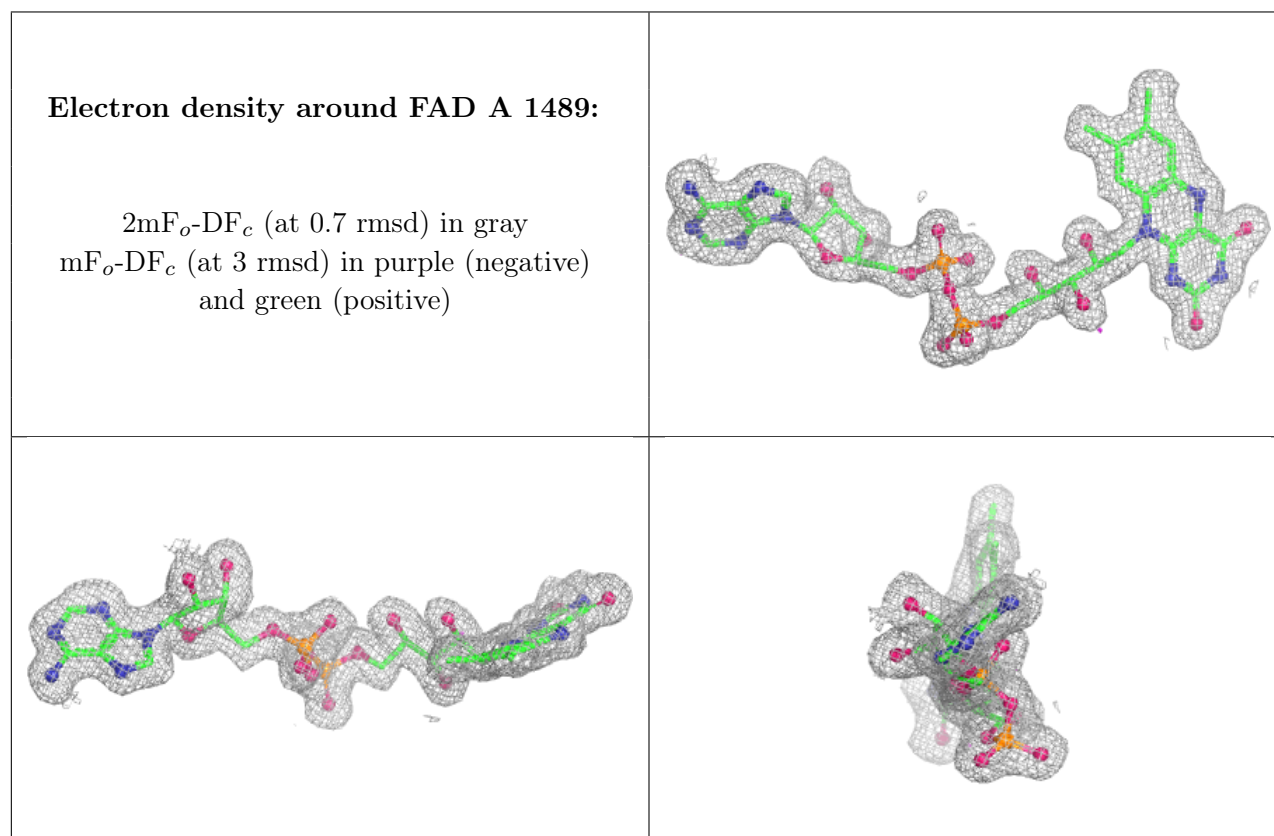
There are no oligosaccharides in this entry.

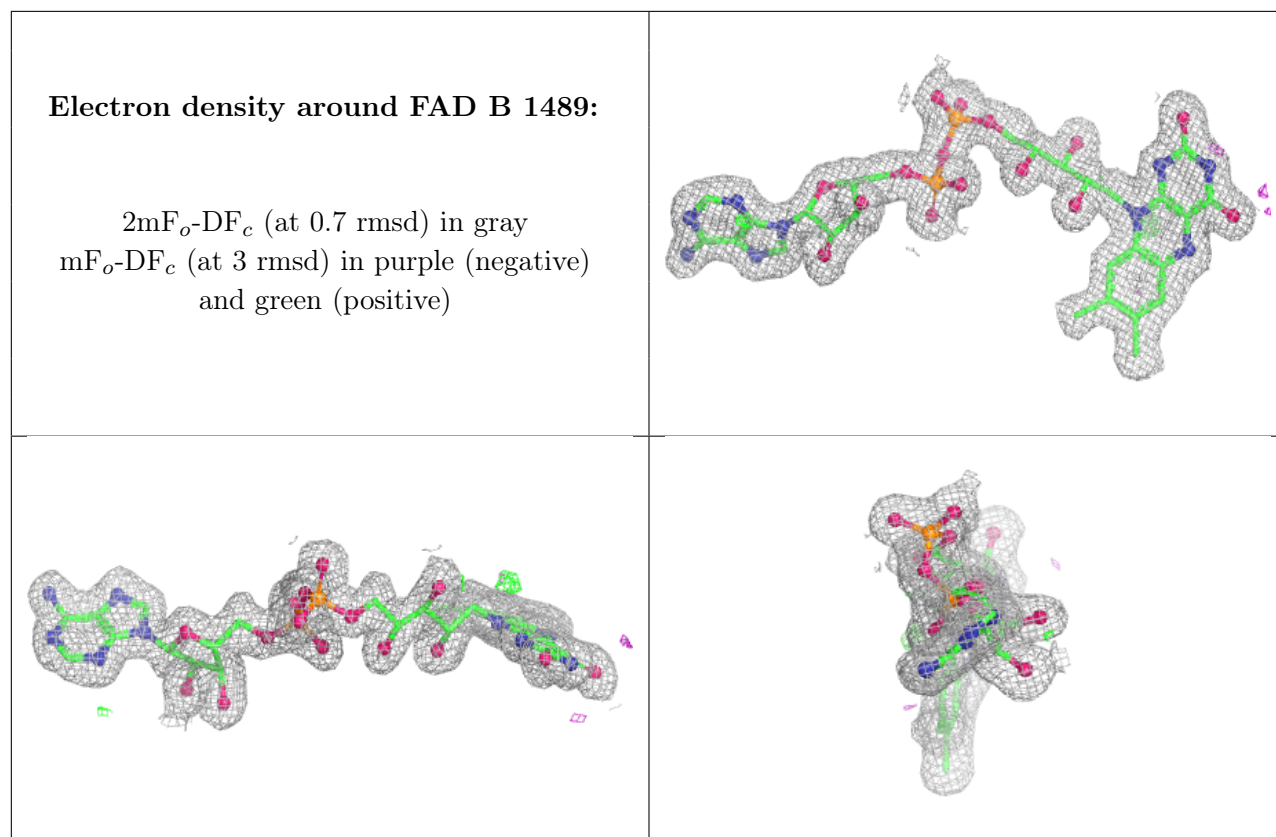
6.4 Ligands [i](#)

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
3	BE2	A	1490	10/10	0.57	0.20	42,43,43,44	0
3	BE2	B	1490	10/10	0.63	0.17	43,45,45,46	0
2	FAD	A	1489	53/53	0.98	0.04	9,12,14,15	0
2	FAD	B	1489	53/53	0.98	0.04	8,12,14,15	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.