



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:30 PM UTC

PDB ID : 2YR4 / pdb_00002yr4
Title : Crystal structure of L-phenylalanine oxiase from Psuedomonas sp. P-501
Authors : Ida, K.; Kurabayashi, M.; Suguro, M.; Suzuki, H.
Deposited on : 2007-04-02
Resolution : 1.70 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

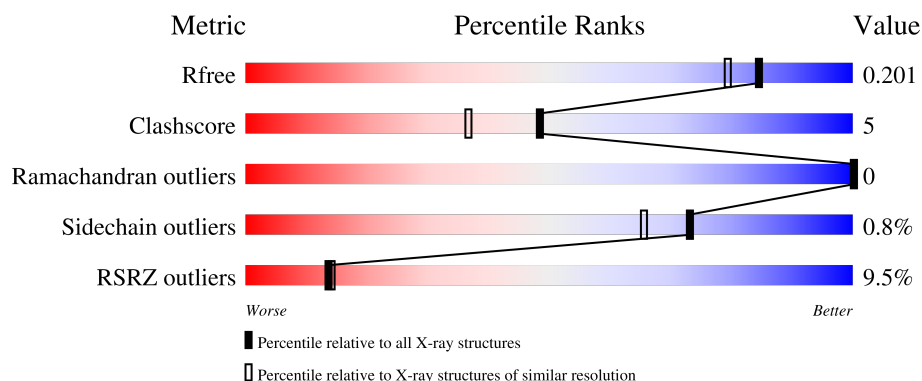
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	721	9% 85% 8% 7%
1	B	721	9% 85% 8% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11927 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 Pro-enzyme of L-phenylalanine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5145	3284	892	958	11			
1	B	673	Total	C	N	O	S	0	0	0
			5145	3287	894	953	11			

There are 16 discrepancies between the modelled and reference sequences:

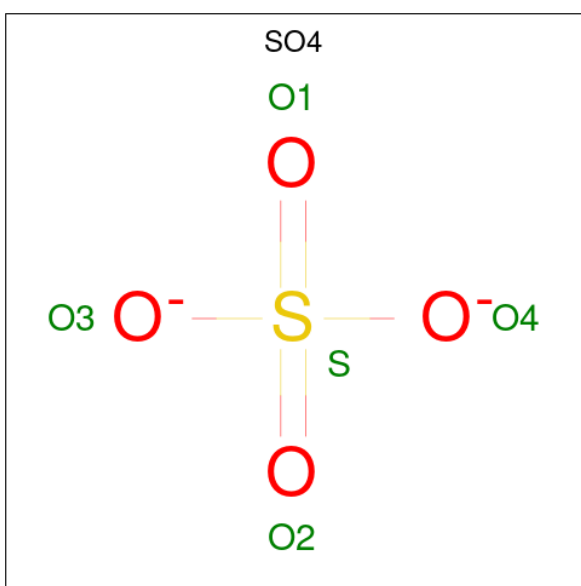
Chain	Residue	Modelled	Actual	Comment	Reference
A	714	LEU	-	expression tag	UNP Q5W9R9
A	715	GLU	-	expression tag	UNP Q5W9R9
A	716	HIS	-	expression tag	UNP Q5W9R9
A	717	HIS	-	expression tag	UNP Q5W9R9
A	718	HIS	-	expression tag	UNP Q5W9R9
A	719	HIS	-	expression tag	UNP Q5W9R9
A	720	HIS	-	expression tag	UNP Q5W9R9
A	721	HIS	-	expression tag	UNP Q5W9R9
B	714	LEU	-	expression tag	UNP Q5W9R9
B	715	GLU	-	expression tag	UNP Q5W9R9
B	716	HIS	-	expression tag	UNP Q5W9R9
B	717	HIS	-	expression tag	UNP Q5W9R9
B	718	HIS	-	expression tag	UNP Q5W9R9
B	719	HIS	-	expression tag	UNP Q5W9R9
B	720	HIS	-	expression tag	UNP Q5W9R9
B	721	HIS	-	expression tag	UNP Q5W9R9

- 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 SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

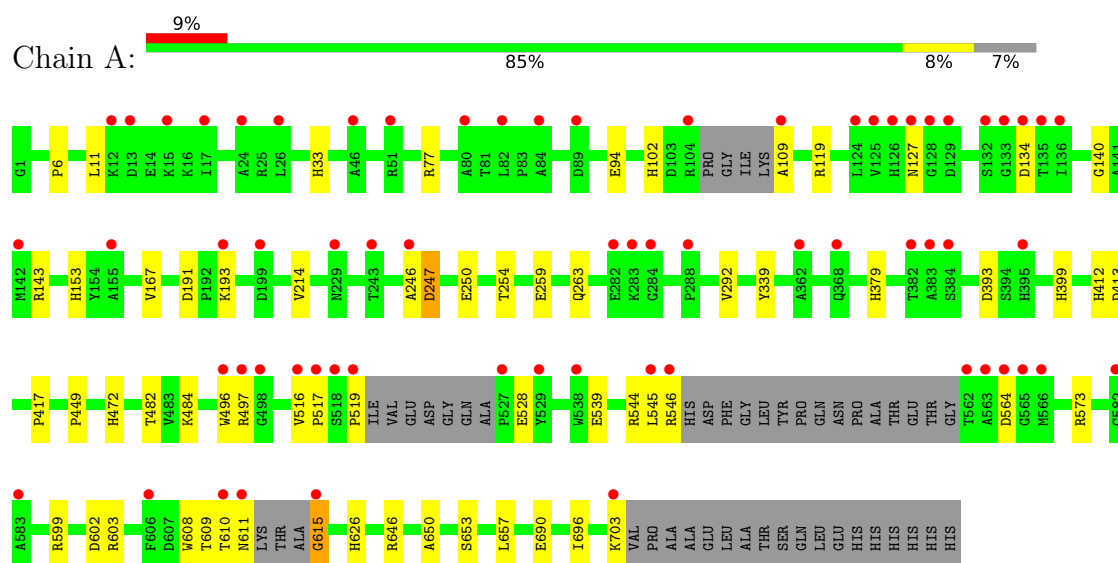
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	755	Total 755	O 755	0	0
4	B	771	Total 771	O 771	0	0

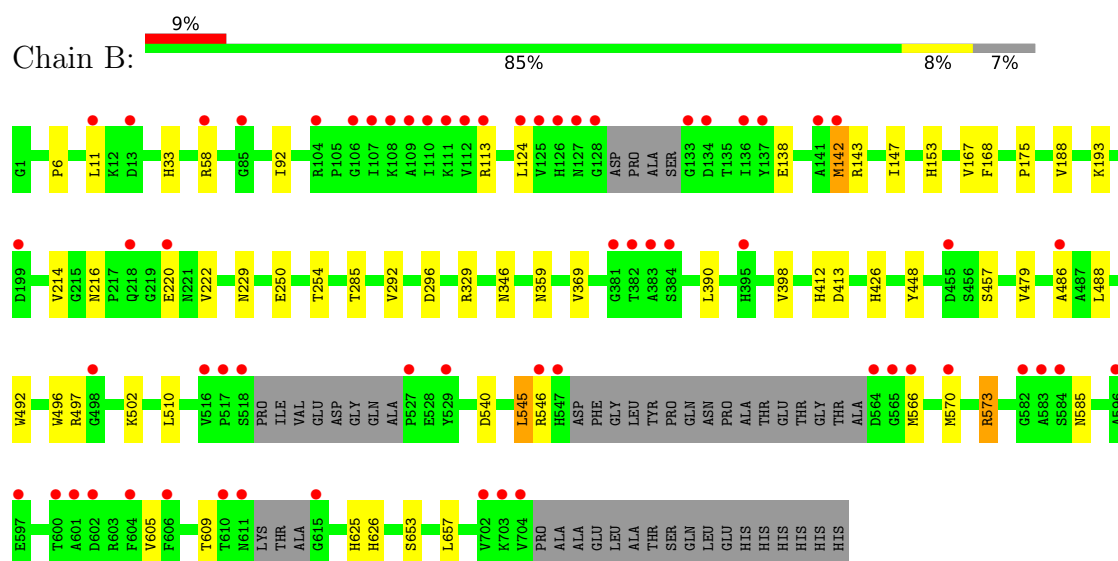
3 Residue-property plots [i](#)

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: Pro-enzyme of L-phenylalanine oxidase



- Molecule 1: Pro-enzyme of L-phenylalanine oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	141.58Å 145.41Å 82.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.77 – 1.70 50.77 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.77-1.70) 99.3 (50.77-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.166 , 0.195 0.175 , 0.201	Depositor DCC
R_{free} test set	9271 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11927	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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, SO4

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	0.96	1/5273 (0.0%)	0.94	2/7189 (0.0%)
1	B	0.95	0/5273	0.90	0/7186
All	All	0.96	1/10546 (0.0%)	0.92	2/14375 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	650	ALA	CA-CB	5.07	1.59	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	615	GLY	CA-C-N	5.06	125.93	121.58
1	A	615	GLY	C-N-CA	5.06	125.93	121.58

There are no chirality outliers.

There are no planarity outliers.

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	5145	0	5060	62	0
1	B	5145	0	5070	55	0
2	A	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	2	0
3	B	5	0	0	0	0
4	A	755	0	0	23	0
4	B	771	0	0	16	0
All	All	11927	0	10192	113	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 5.

All (113) 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:127:ASN:HD21	1:A:599:ARG:NH2	1.44	1.14
1:A:127:ASN:HD21	1:A:599:ARG:CZ	1.87	0.86
1:B:479:VAL:HG21	1:B:570:MET:SD	2.19	0.83
1:B:143:ARG:NH1	2:B:801:FAD:O4	2.14	0.81
1:A:379:HIS:HE1	1:A:646:ARG:H	1.30	0.79
1:A:519:PRO:HA	4:A:1513:HOH:O	1.81	0.79
1:A:127:ASN:ND2	1:A:599:ARG:NH2	2.29	0.73
1:A:545:LEU:HD21	1:A:573:ARG:HG3	1.73	0.71
1:A:143:ARG:NH1	2:A:801:FAD:O4	2.24	0.70
1:A:496:TRP:CD1	1:A:497:ARG:HG2	2.25	0.70
1:A:472:HIS:HD2	1:B:540:ASP:OD2	1.75	0.69
1:A:134:ASP:O	4:A:1503:HOH:O	2.11	0.69
1:B:11:LEU:HD11	1:B:167:VAL:HG11	1.74	0.68
1:A:11:LEU:HD11	1:A:167:VAL:HG11	1.75	0.67
1:B:113:ARG:C	1:B:124:LEU:HD11	2.21	0.66
1:A:696:ILE:HD11	4:A:1259:HOH:O	1.96	0.65
1:B:412:HIS:HD2	1:B:653:SER:OG	1.80	0.64
1:A:412:HIS:HD2	1:A:653:SER:OG	1.80	0.64
1:B:58:ARG:HD2	4:B:2514:HOH:O	1.96	0.64
1:B:329:ARG:HH22	1:B:625:HIS:HD2	1.42	0.64
1:A:127:ASN:ND2	1:A:599:ARG:CZ	2.60	0.62
1:B:216:ASN:HB3	4:B:2664:HOH:O	2.00	0.61
1:A:393:ASP:OD2	1:A:399:HIS:HE1	1.83	0.61
1:A:472:HIS:HE1	1:A:539:GLU:OE2	1.84	0.60
1:A:690:GLU:HG3	4:A:1245:HOH:O	2.00	0.60
1:A:545:LEU:CD2	1:A:573:ARG:HG3	2.32	0.58
1:B:142:MET:CE	1:B:168:PHE:CZ	2.86	0.58
1:A:6:PRO:HB3	1:A:214:VAL:HG21	1.84	0.58
1:A:484:LYS:NZ	1:A:528:GLU:OE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:THR:HG21	1:A:599:ARG:HH21	1.69	0.58
1:B:488:LEU:HD13	1:B:502:LYS:HE2	1.86	0.57
1:B:329:ARG:HH22	1:B:625:HIS:CD2	2.21	0.57
1:A:413:ASP:HB2	4:A:1489:HOH:O	2.05	0.57
1:B:113:ARG:O	1:B:124:LEU:HD11	2.05	0.56
1:A:615:GLY:C	4:A:1444:HOH:O	2.50	0.55
1:A:546:ARG:C	4:A:1258:HOH:O	2.50	0.54
1:B:175:PRO:HA	1:B:188:VAL:HG22	1.88	0.54
1:B:216:ASN:HD21	1:B:222:VAL:CG1	2.21	0.54
1:A:246:ALA:O	1:A:247:ASP:HB2	2.08	0.54
1:B:216:ASN:ND2	1:B:222:VAL:HG13	2.23	0.53
1:B:142:MET:CE	1:B:168:PHE:CE1	2.92	0.53
1:B:585:ASN:HA	4:B:2246:HOH:O	2.07	0.53
2:B:801:FAD:H9	2:B:801:FAD:O2'	2.09	0.52
1:A:250:GLU:OE2	1:A:254:THR:HG21	2.10	0.52
1:A:609:THR:C	4:A:1445:HOH:O	2.52	0.52
1:A:77:ARG:HD3	4:A:962:HOH:O	2.09	0.52
1:A:379:HIS:CE1	1:A:646:ARG:H	2.19	0.52
1:B:413:ASP:HB2	4:B:2716:HOH:O	2.09	0.51
1:B:566:MET:HG2	1:B:605:VAL:HG11	1.91	0.51
1:B:359:ASN:HB2	4:B:2717:HOH:O	2.09	0.51
1:A:153:HIS:HE1	4:A:956:HOH:O	1.94	0.51
1:A:573:ARG:HD3	4:A:1485:HOH:O	2.11	0.51
1:B:33:HIS:CE1	1:B:657:LEU:HD11	2.47	0.51
1:A:94:GLU:O	1:A:102:HIS:HE1	1.94	0.50
1:B:250:GLU:OE2	1:B:254:THR:HG21	2.11	0.50
1:A:626:HIS:HE1	4:A:1031:HOH:O	1.94	0.50
1:B:142:MET:HE3	1:B:168:PHE:CZ	2.46	0.50
1:B:124:LEU:HD22	4:B:2727:HOH:O	2.10	0.49
1:B:626:HIS:HE1	4:B:2103:HOH:O	1.95	0.49
1:B:486:ALA:HB3	4:B:2731:HOH:O	2.12	0.49
1:B:496:TRP:CD1	1:B:497:ARG:HG2	2.47	0.49
1:A:703:LYS:HE3	1:B:292:VAL:HG13	1.93	0.49
4:A:1198:HOH:O	1:B:626:HIS:HD2	1.96	0.48
1:A:646:ARG:CZ	4:A:1488:HOH:O	2.60	0.48
1:B:6:PRO:HB3	1:B:214:VAL:HG21	1.96	0.48
1:A:33:HIS:CE1	1:A:657:LEU:HD11	2.49	0.48
1:B:142:MET:HE3	1:B:168:PHE:CE1	2.48	0.48
1:A:482:THR:HG21	1:A:599:ARG:NH2	2.28	0.47
1:B:285:THR:O	1:B:285:THR:HG22	2.14	0.47
1:B:193:LYS:NZ	4:B:2772:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:HIS:HD2	1:B:296:ASP:OD2	1.97	0.47
1:A:519:PRO:CG	4:A:1508:HOH:O	2.62	0.47
1:B:566:MET:HE3	1:B:570:MET:HG3	1.96	0.47
1:A:615:GLY:N	4:A:1204:HOH:O	2.48	0.46
1:A:102:HIS:HD2	4:A:1093:HOH:O	1.98	0.46
1:A:610:THR:O	1:A:610:THR:HG22	2.15	0.46
1:A:167:VAL:HG22	1:A:339:TYR:CE1	2.50	0.46
1:B:573:ARG:NH2	4:B:2159:HOH:O	2.49	0.45
1:A:259:GLU:O	1:A:263:GLN:HG3	2.16	0.45
1:A:412:HIS:CD2	1:A:653:SER:OG	2.66	0.45
1:B:153:HIS:HE1	4:B:2087:HOH:O	1.99	0.45
1:A:609:THR:O	1:B:609:THR:O	2.35	0.44
1:B:492:TRP:HE3	4:B:2415:HOH:O	2.00	0.44
1:A:246:ALA:O	1:A:247:ASP:CB	2.66	0.44
2:A:801:FAD:O2'	2:A:801:FAD:H9	2.18	0.44
1:B:546:ARG:NH1	4:B:2666:HOH:O	2.42	0.44
1:A:564:ASP:OD1	1:A:603:ARG:NH1	2.52	0.43
1:B:216:ASN:ND2	1:B:222:VAL:CG1	2.81	0.43
1:A:191:ASP:OD1	1:A:193:LYS:HD3	2.18	0.43
1:A:544:ARG:NH2	4:A:855:HOH:O	2.50	0.43
1:B:412:HIS:HE1	4:B:2177:HOH:O	2.01	0.43
1:B:147:ILE:HD12	4:B:2356:HOH:O	2.19	0.43
1:A:608:TRP:O	1:B:546:ARG:NH2	2.53	0.42
1:A:127:ASN:ND2	1:A:602:ASP:OD2	2.52	0.42
1:A:127:ASN:OD1	1:A:127:ASN:O	2.37	0.42
1:A:292:VAL:HG21	1:B:457:SER:HB2	2.01	0.42
1:B:545:LEU:HD22	1:B:573:ARG:CZ	2.50	0.42
1:B:113:ARG:HB3	1:B:124:LEU:HD21	2.02	0.42
1:A:119:ARG:O	1:A:140:GLY:HA3	2.20	0.42
1:A:413:ASP:HB2	4:A:850:HOH:O	2.19	0.42
1:B:426:HIS:HB2	1:B:448:TYR:CE1	2.54	0.42
1:A:109:ALA:HB1	4:A:1550:HOH:O	2.20	0.41
1:A:516:VAL:HG13	1:A:517:PRO:HD2	2.01	0.41
1:A:703:LYS:CE	4:A:1411:HOH:O	2.68	0.41
1:B:390:LEU:HD11	1:B:398:VAL:CG2	2.51	0.41
1:A:703:LYS:HE3	4:A:1411:HOH:O	2.19	0.41
1:B:175:PRO:CA	1:B:188:VAL:HG22	2.50	0.41
1:B:92:ILE:CG2	1:B:369:VAL:HG22	2.51	0.41
1:A:417:PRO:HB2	4:A:1085:HOH:O	2.21	0.41
1:B:142:MET:CE	1:B:143:ARG:HD2	2.51	0.41
1:A:379:HIS:HD2	1:A:449:PRO:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ASP:HB2	4:B:2187:HOH:O	2.20	0.41
1:B:138:GLU:CD	1:B:346:ASN:HD22	2.30	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	664/721 (92%)	648 (98%)	16 (2%)	0	100	100
1	B	663/721 (92%)	649 (98%)	14 (2%)	0	100	100
All	All	1327/1442 (92%)	1297 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	529/566 (94%)	527 (100%)	2 (0%)	84	80
1	B	529/566 (94%)	523 (99%)	6 (1%)	65	54
All	All	1058/1132 (94%)	1050 (99%)	8 (1%)	73	65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	ASP
1	A	611	ASN
1	B	142	MET
1	B	220	GLU
1	B	229	ASN
1	B	510	LEU
1	B	545	LEU
1	B	573	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	102	HIS
1	A	127	ASN
1	A	153	HIS
1	A	170	ASN
1	A	263	GLN
1	A	379	HIS
1	A	399	HIS
1	A	412	HIS
1	A	472	HIS
1	A	495	GLN
1	A	587	GLN
1	A	611	ASN
1	A	626	HIS
1	A	670	ASN
1	B	153	HIS
1	B	216	ASN
1	B	263	GLN
1	B	321	ASN
1	B	346	ASN
1	B	376	ASN
1	B	412	HIS
1	B	442	HIS
1	B	445	ASN
1	B	446	GLN
1	B	470	GLN
1	B	593	GLN
1	B	625	HIS
1	B	626	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	2001	-	4,4,4	0.30	0	6,6,6	0.30	0
2	FAD	B	801	-	58,58,58	1.33	8 (13%)	85,89,89	1.75	17 (20%)
2	FAD	A	801	-	58,58,58	1.45	11 (18%)	85,89,89	1.76	19 (22%)

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	801	-	-	3/34/50/50	0/6/6/6
2	FAD	A	801	-	-	5/34/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	C4X-N5	4.33	1.40	1.30
2	B	801	FAD	C4X-C10	-3.58	1.33	1.44
2	A	801	FAD	C9A-C5X	-3.29	1.36	1.41
2	A	801	FAD	C4X-C10	-3.15	1.34	1.44
2	B	801	FAD	C4X-N5	3.13	1.37	1.30
2	A	801	FAD	C2A-N3A	2.98	1.39	1.33
2	B	801	FAD	C9A-C5X	-2.77	1.36	1.41
2	A	801	FAD	C10-N1	2.56	1.38	1.33
2	B	801	FAD	C2A-N3A	2.35	1.38	1.33
2	A	801	FAD	C1'-N10	2.35	1.53	1.47
2	B	801	FAD	C4X-C4	-2.31	1.36	1.44
2	A	801	FAD	PA-O3P	2.27	1.61	1.59
2	A	801	FAD	C1'-C2'	-2.27	1.49	1.52
2	A	801	FAD	C2-N3	-2.26	1.34	1.39
2	A	801	FAD	C8M-C8	2.22	1.55	1.51
2	B	801	FAD	C4A-N3A	2.13	1.38	1.34
2	B	801	FAD	O2-C2	-2.03	1.20	1.24
2	B	801	FAD	C2-N1	-2.03	1.32	1.36
2	A	801	FAD	O4B-C4B	-2.02	1.40	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	C9A-C5X-N5	-5.48	116.64	122.45
2	A	801	FAD	C5A-C4A-N3A	-5.00	119.83	126.72
2	A	801	FAD	C6A-C5A-C4A	4.68	123.56	117.18
2	B	801	FAD	C4-N3-C2	-4.51	117.63	125.64
2	B	801	FAD	C5A-C4A-N3A	-4.42	120.63	126.72
2	B	801	FAD	O4-C4-C4X	-4.30	115.17	126.53
2	A	801	FAD	C9A-C5X-N5	-4.28	117.91	122.45
2	B	801	FAD	C4X-C4-N3	4.27	124.12	113.25
2	B	801	FAD	C10-N1-C2	3.77	125.01	116.85
2	A	801	FAD	C4X-C4-N3	3.73	122.74	113.25
2	A	801	FAD	C4-C4X-N5	3.70	123.31	118.21
2	B	801	FAD	N3A-C4A-N9A	3.46	133.06	127.17
2	A	801	FAD	C4-N3-C2	-3.37	119.66	125.64
2	B	801	FAD	C5X-C9A-N10	3.26	120.91	117.97
2	A	801	FAD	N9A-C8A-N7A	-3.24	109.33	113.94
2	A	801	FAD	N3A-C4A-N9A	3.23	132.67	127.17
2	A	801	FAD	C5A-N7A-C8A	3.13	108.36	103.45
2	B	801	FAD	N9A-C8A-N7A	-2.96	109.73	113.94
2	B	801	FAD	C5'-C4'-C3'	-2.96	106.63	112.22
2	B	801	FAD	C7M-C7-C8	-2.90	114.83	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	C10-N1-C2	2.82	122.95	116.85
2	A	801	FAD	C7M-C7-C8	-2.81	115.03	120.76
2	A	801	FAD	C6-C5X-N5	2.61	122.78	118.44
2	B	801	FAD	C8M-C8-C9	-2.61	114.97	119.57
2	A	801	FAD	C9A-C9-C8	2.59	124.42	119.22
2	A	801	FAD	C4'-C3'-C2'	2.48	117.70	113.57
2	B	801	FAD	C6-C5X-N5	2.42	122.46	118.44
2	B	801	FAD	C4-C4X-N5	2.34	121.43	118.21
2	B	801	FAD	C6A-C5A-C4A	2.30	120.32	117.18
2	A	801	FAD	C7M-C7-C6	2.26	123.56	119.57
2	A	801	FAD	C4A-C5A-N7A	-2.22	108.05	110.58
2	A	801	FAD	C5'-C4'-C3'	-2.18	108.11	112.22
2	A	801	FAD	O4-C4-C4X	-2.18	120.79	126.53
2	B	801	FAD	C7M-C7-C6	2.17	123.41	119.57
2	B	801	FAD	C5A-N7A-C8A	2.16	106.85	103.45
2	A	801	FAD	C1'-N10-C9A	-2.10	116.55	120.63

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FAD	PA-O3P-P-O5'
2	B	801	FAD	PA-O3P-P-O5'
2	A	801	FAD	C2'-C3'-C4'-O4'
2	B	801	FAD	C2'-C3'-C4'-O4'
2	A	801	FAD	C2'-C3'-C4'-C5'
2	A	801	FAD	O3'-C3'-C4'-O4'
2	A	801	FAD	O3'-C3'-C4'-C5'
2	B	801	FAD	C2'-C3'-C4'-C5'

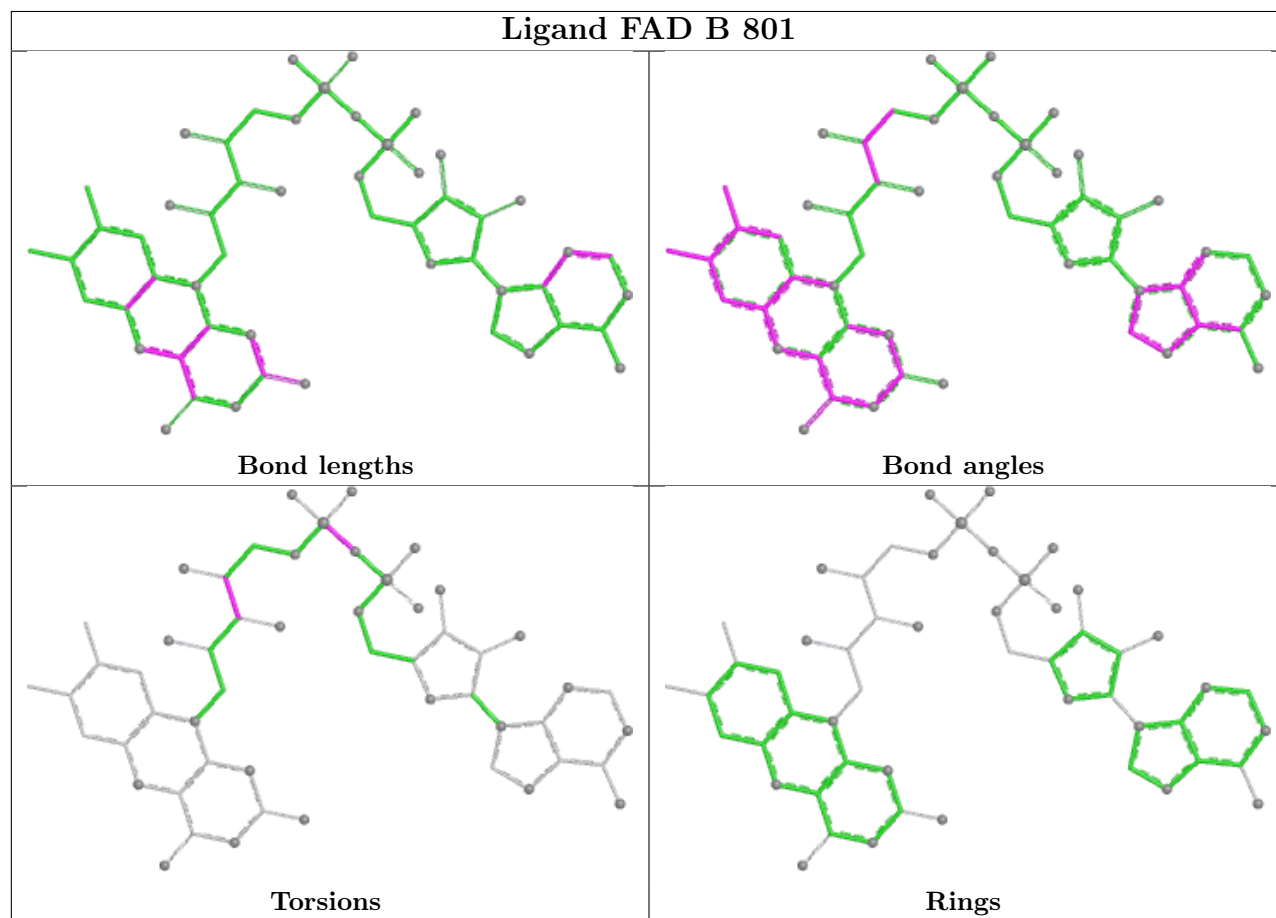
There are no ring outliers.

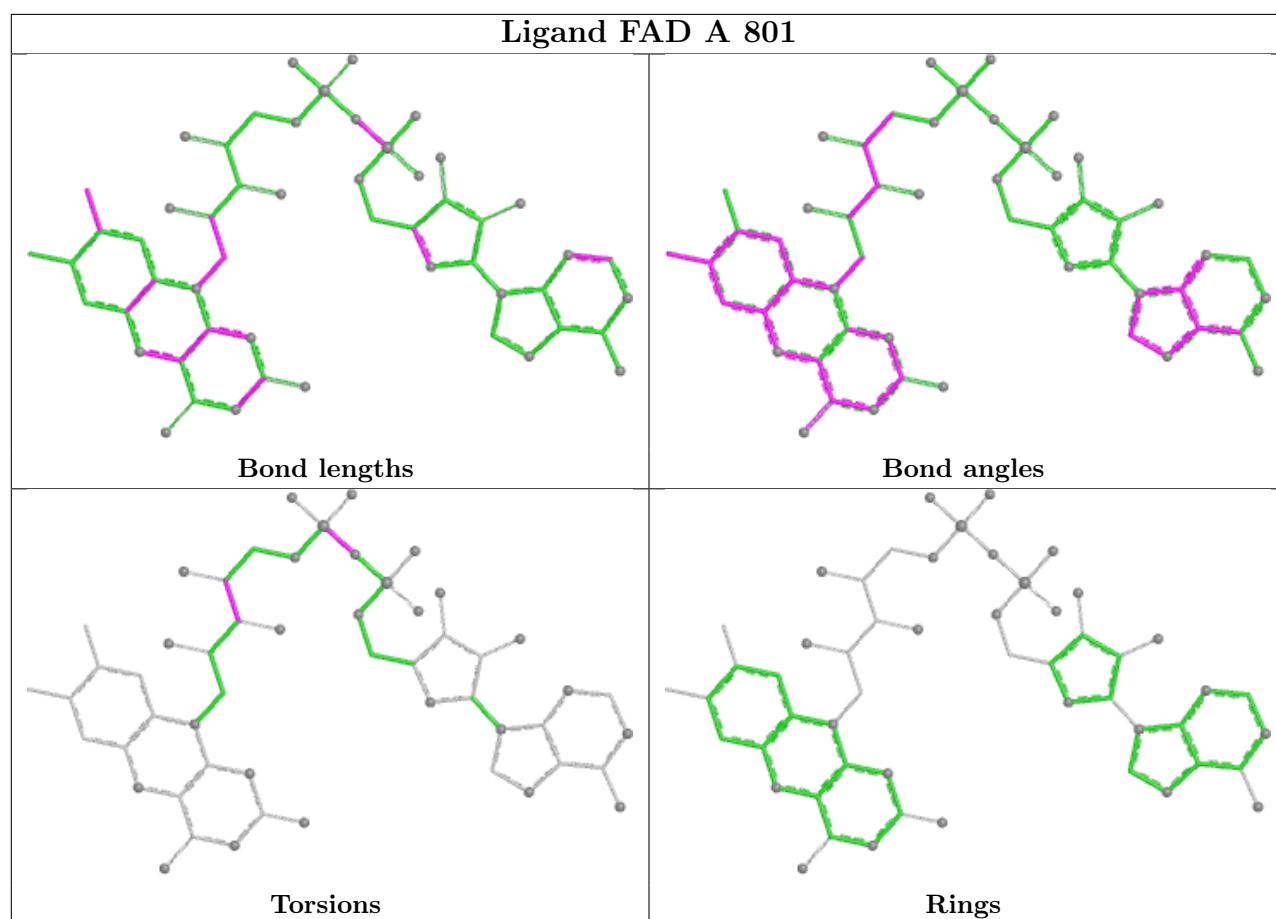
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	FAD	2	0
2	A	801	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	674/721 (93%)	0.52	66 (9%)	13 13	12, 23, 38, 53	0
1	B	673/721 (93%)	0.33	62 (9%)	14 15	11, 20, 41, 62	0
All	All	1347/1442 (93%)	0.42	128 (9%)	14 14	11, 22, 39, 62	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	ALA	5.9
1	A	246	ALA	5.9
1	B	125	VAL	5.8
1	B	518	SER	5.5
1	B	133	GLY	5.3
1	A	610	THR	5.0
1	A	519	PRO	5.0
1	B	110	ILE	4.9
1	B	112	VAL	4.9
1	A	13	ASP	4.8
1	A	563	ALA	4.8
1	A	582	GLY	4.7
1	A	128	GLY	4.7
1	A	127	ASN	4.6
1	B	220	GLU	4.4
1	A	518	SER	4.2
1	A	562	THR	4.2
1	B	136	ILE	4.1
1	B	126	HIS	4.0
1	B	602	ASP	3.9
1	B	606	PHE	3.9
1	A	104	ARG	3.9
1	B	128	GLY	3.9
1	A	583	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	124	LEU	3.8
1	B	104	ARG	3.7
1	A	615	GLY	3.7
1	B	583	ALA	3.7
1	B	547	HIS	3.7
1	B	11	LEU	3.7
1	B	134	ASP	3.6
1	B	517	PRO	3.5
1	B	107	ILE	3.5
1	A	498	GLY	3.5
1	A	126	HIS	3.5
1	A	516	VAL	3.5
1	B	565	GLY	3.4
1	B	601	ALA	3.4
1	A	545	LEU	3.4
1	B	600	THR	3.3
1	B	218	GLN	3.3
1	B	137	TYR	3.3
1	B	584	SER	3.3
1	A	362	ALA	3.2
1	A	133	GLY	3.2
1	A	132	SER	3.1
1	B	141	ALA	3.1
1	A	546	ARG	3.1
1	B	85	GLY	3.1
1	B	142	MET	3.1
1	B	570	MET	3.1
1	B	111	LYS	3.1
1	A	288	PRO	3.1
1	A	17	ILE	3.1
1	A	611	ASN	3.1
1	B	611	ASN	3.1
1	B	13	ASP	3.1
1	B	529	TYR	3.0
1	B	546	ARG	3.0
1	B	109	ALA	3.0
1	A	129	ASP	3.0
1	B	564	ASP	3.0
1	B	703	LYS	3.0
1	B	610	THR	2.9
1	B	704	VAL	2.9
1	A	384	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	51	ARG	2.8
1	B	498	GLY	2.8
1	A	26	LEU	2.8
1	B	384	SER	2.8
1	B	527	PRO	2.8
1	B	108	LYS	2.8
1	A	497	ARG	2.7
1	A	125	VAL	2.7
1	A	82	LEU	2.7
1	B	106	GLY	2.7
1	A	229	ASN	2.7
1	A	383	ALA	2.7
1	B	383	ALA	2.7
1	A	517	PRO	2.7
1	A	538	TRP	2.7
1	A	199	ASP	2.7
1	A	527	PRO	2.6
1	B	615	GLY	2.6
1	A	80	ALA	2.6
1	A	703	LYS	2.6
1	A	566	MET	2.6
1	A	382	THR	2.6
1	B	113	ARG	2.6
1	B	597	GLU	2.6
1	A	89	ASP	2.5
1	B	604	PHE	2.5
1	A	496	TRP	2.5
1	A	368	GLN	2.5
1	B	596	ALA	2.5
1	A	135	THR	2.5
1	A	243	THR	2.5
1	B	127	ASN	2.4
1	A	15	LYS	2.4
1	A	529	TYR	2.4
1	A	564	ASP	2.4
1	A	142	MET	2.4
1	B	566	MET	2.4
1	A	124	LEU	2.4
1	B	381	GLY	2.4
1	A	565	GLY	2.4
1	A	284	GLY	2.3
1	A	282	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	382	THR	2.3
1	A	24	ALA	2.3
1	A	134	ASP	2.3
1	A	136	ILE	2.3
1	B	199	ASP	2.3
1	A	395	HIS	2.2
1	B	486	ALA	2.2
1	B	582	GLY	2.2
1	A	12	LYS	2.2
1	B	702	VAL	2.2
1	B	455	ASP	2.2
1	B	395	HIS	2.2
1	A	155	ALA	2.1
1	A	46	ALA	2.1
1	A	193	LYS	2.1
1	A	283	LYS	2.1
1	B	58	ARG	2.0
1	B	516	VAL	2.0
1	A	606	PHE	2.0
1	A	84	ALA	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](#)

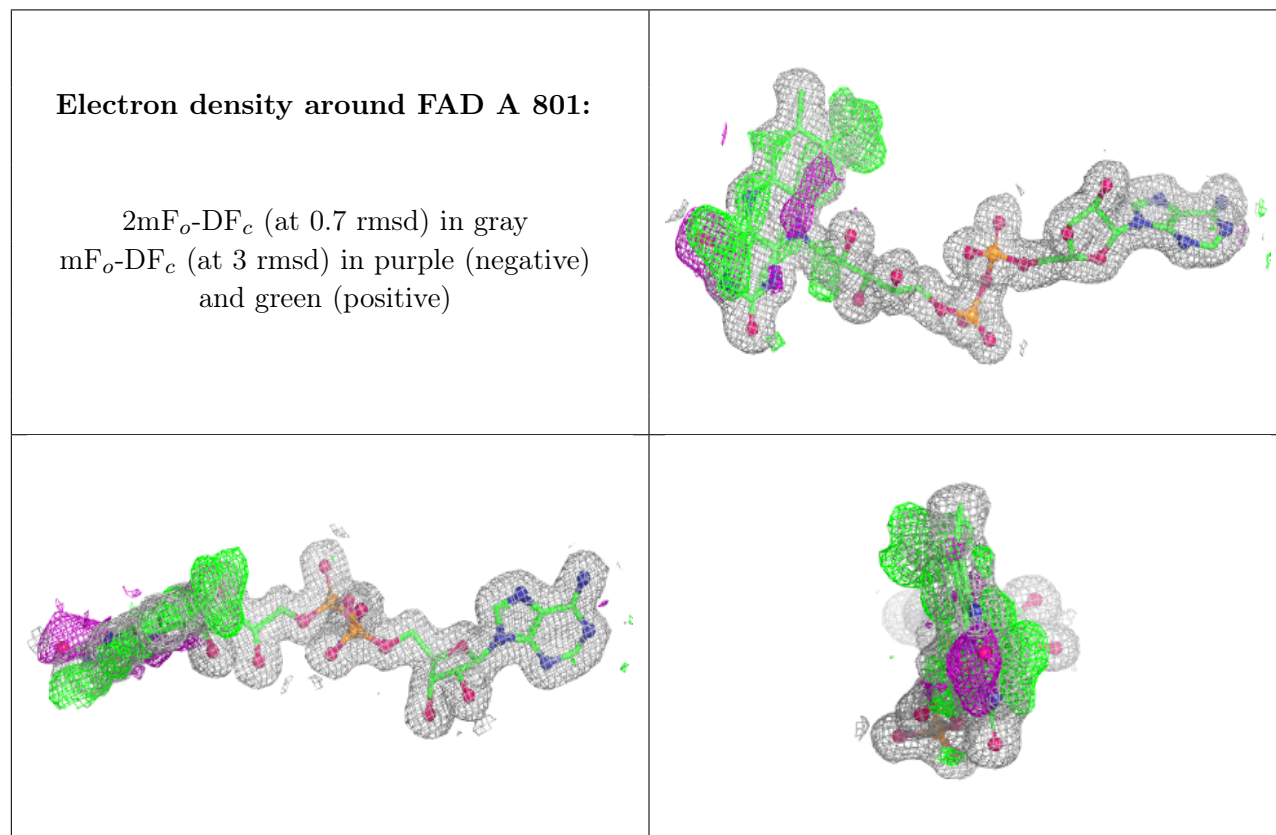
There are no oligosaccharides in this entry.

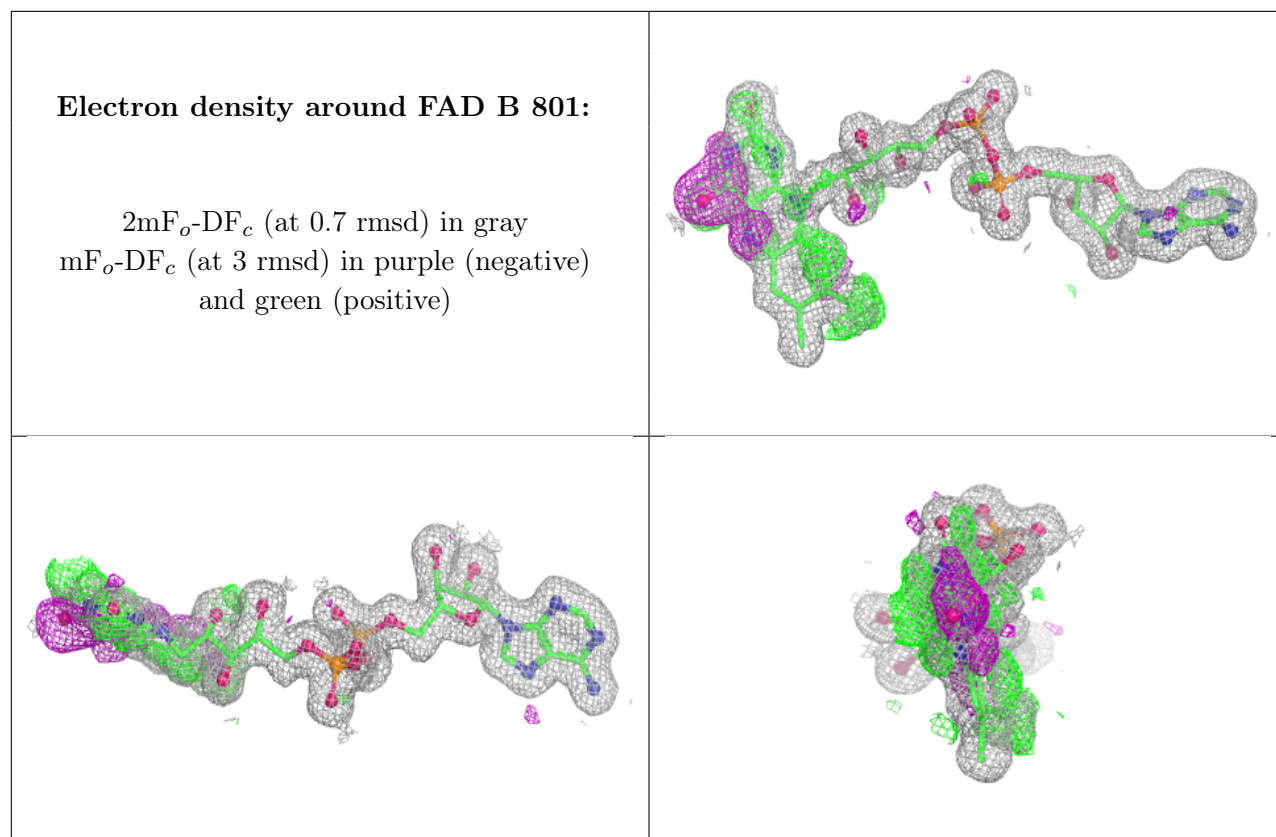
6.4 Ligands [i](#)

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
3	SO4	B	2001	5/5	0.84	0.14	59,60,61,61	0
2	FAD	A	801	53/53	0.93	0.09	12,16,22,29	0
2	FAD	B	801	53/53	0.94	0.09	11,15,22,29	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.