Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2025 – 12:08 am GMT

PDB ID	:	9H5Q
Title	:	Crystal structure of Thermoanaerobacterales bacterium monoamine oxidase in complex with spermidine and its oxidation products
Authors	:	Basile, L.; Poli, C.; Santema, L.L.; Lesenciuc, R.C.; Fraaije, M.W.; Binda, C.
Deposited on	:	2024-10-23
Resolution	:	1.80 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:

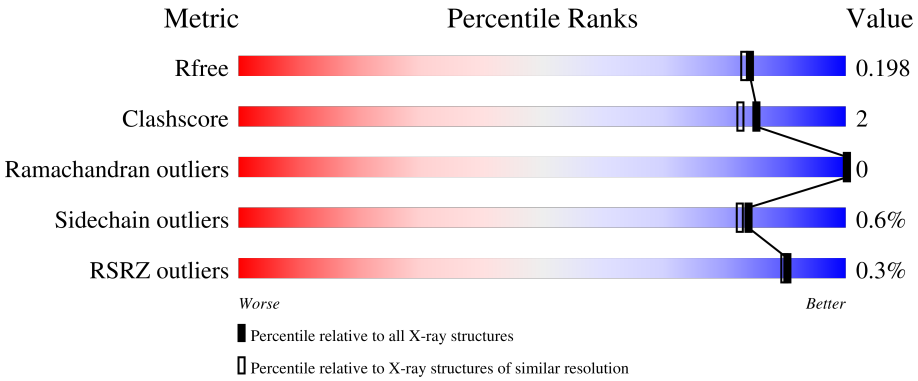
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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 <=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	474	88% 6% 5%
1	B	474	% 90% 5% 5%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7392 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 Monoamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	2	0
			3361	2112	610	634	5			
1	B	450	Total	C	N	O	S	0	0	0
			3365	2113	609	639	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0AAJ6N6J2
A	-19	GLY	-	expression tag	UNP A0AAJ6N6J2
A	-18	SER	-	expression tag	UNP A0AAJ6N6J2
A	-17	SER	-	expression tag	UNP A0AAJ6N6J2
A	-16	HIS	-	expression tag	UNP A0AAJ6N6J2
A	-15	HIS	-	expression tag	UNP A0AAJ6N6J2
A	-14	HIS	-	expression tag	UNP A0AAJ6N6J2
A	-13	HIS	-	expression tag	UNP A0AAJ6N6J2
A	-12	HIS	-	expression tag	UNP A0AAJ6N6J2
A	-11	HIS	-	expression tag	UNP A0AAJ6N6J2
A	-10	GLY	-	expression tag	UNP A0AAJ6N6J2
A	-9	SER	-	expression tag	UNP A0AAJ6N6J2
A	-8	GLY	-	expression tag	UNP A0AAJ6N6J2
A	-7	LEU	-	expression tag	UNP A0AAJ6N6J2
A	-6	VAL	-	expression tag	UNP A0AAJ6N6J2
A	-5	PRO	-	expression tag	UNP A0AAJ6N6J2
A	-4	ARG	-	expression tag	UNP A0AAJ6N6J2
A	-3	GLY	-	expression tag	UNP A0AAJ6N6J2
A	-2	SER	-	expression tag	UNP A0AAJ6N6J2
A	-1	ALA	-	expression tag	UNP A0AAJ6N6J2
A	0	GLY	-	expression tag	UNP A0AAJ6N6J2
B	-20	MET	-	initiating methionine	UNP A0AAJ6N6J2
B	-19	GLY	-	expression tag	UNP A0AAJ6N6J2
B	-18	SER	-	expression tag	UNP A0AAJ6N6J2
B	-17	SER	-	expression tag	UNP A0AAJ6N6J2

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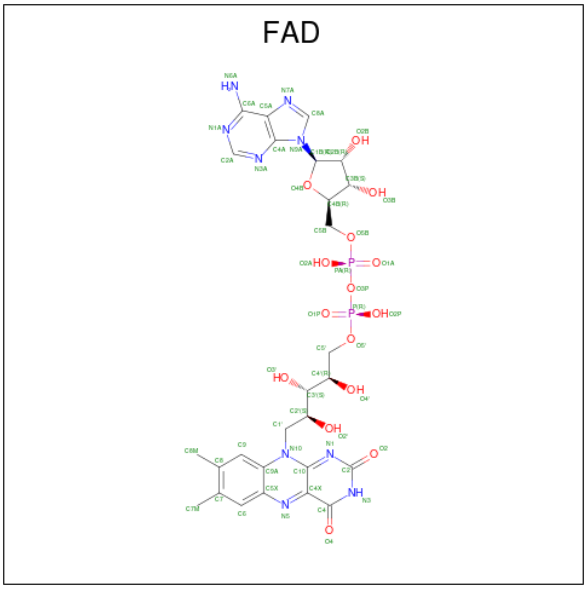
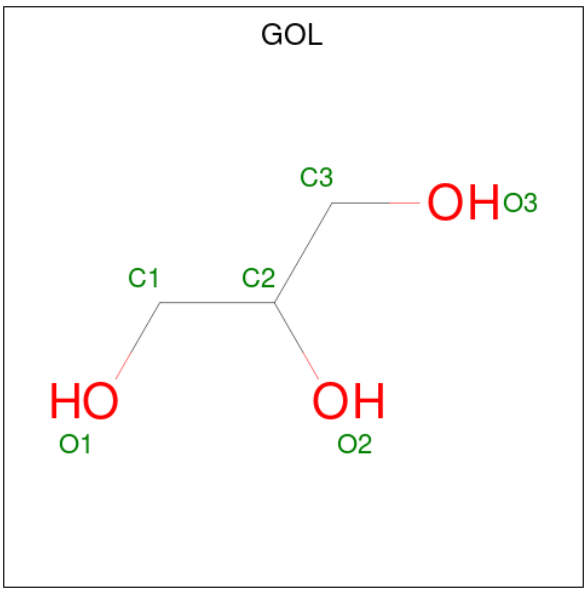
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP A0AAJ6N6J2
B	-15	HIS	-	expression tag	UNP A0AAJ6N6J2
B	-14	HIS	-	expression tag	UNP A0AAJ6N6J2
B	-13	HIS	-	expression tag	UNP A0AAJ6N6J2
B	-12	HIS	-	expression tag	UNP A0AAJ6N6J2
B	-11	HIS	-	expression tag	UNP A0AAJ6N6J2
B	-10	GLY	-	expression tag	UNP A0AAJ6N6J2
B	-9	SER	-	expression tag	UNP A0AAJ6N6J2
B	-8	GLY	-	expression tag	UNP A0AAJ6N6J2
B	-7	LEU	-	expression tag	UNP A0AAJ6N6J2
B	-6	VAL	-	expression tag	UNP A0AAJ6N6J2
B	-5	PRO	-	expression tag	UNP A0AAJ6N6J2
B	-4	ARG	-	expression tag	UNP A0AAJ6N6J2
B	-3	GLY	-	expression tag	UNP A0AAJ6N6J2
B	-2	SER	-	expression tag	UNP A0AAJ6N6J2
B	-1	ALA	-	expression tag	UNP A0AAJ6N6J2
B	0	GLY	-	expression tag	UNP A0AAJ6N6J2

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



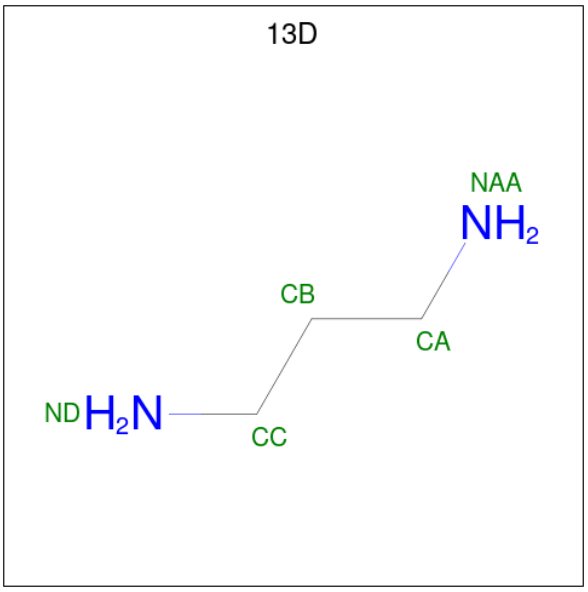
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



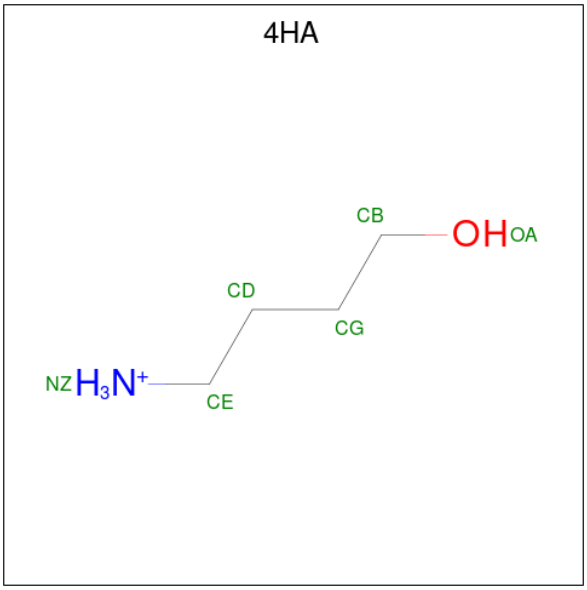
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is 1,3-DIAMINOPROPANE (three-letter code: 13D) (formula: $C_3H_{10}N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 5 3 2	0	0

- Molecule 5 is 4-HYDROXYBUTAN-1-AMINIUM (three-letter code: 4HA) (formula: $C_4H_{12}NO$) (labeled as "Ligand of Interest" by depositor).

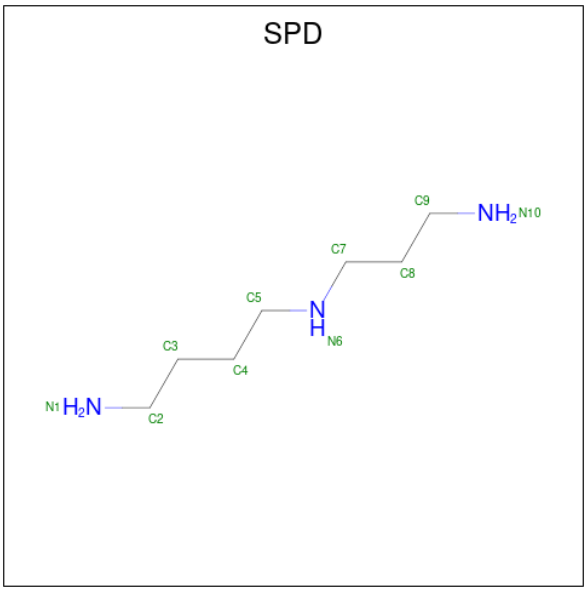


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 6 4 1 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	2	Total Mg 2 2	0	0

- Molecule 7 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is water.

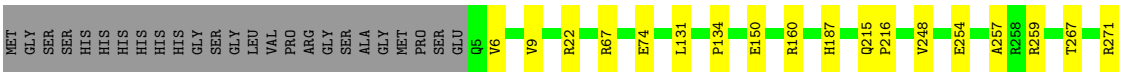
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	274	Total O 274 274	0	0
8	B	244	Total O 244 244	0	0

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.

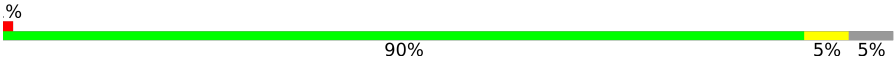
• Molecule 1: Monoamine oxidase

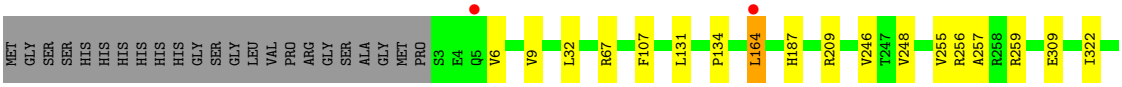
Chain A:

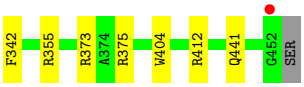


• Molecule 1: Monoamine oxidase

Chain B:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.33Å 94.46Å 127.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.95 – 1.80 63.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (63.95-1.80) 99.7 (63.95-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.154 , 0.189 0.167 , 0.198	Depositor DCC
R_{free} test set	3838 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 29.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7392	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, FAD, SPD, 4HA, GOL, 13D

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	0.80	1/3451 (0.0%)	0.89	6/4727 (0.1%)
1	B	0.79	0/3449	0.87	9/4724 (0.2%)
All	All	0.79	1/6900 (0.0%)	0.88	15/9451 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	GLU	CD-OE1	5.60	1.31	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	ARG	NE-CZ-NH2	-11.59	114.50	120.30
1	A	259	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	412	ARG	CG-CD-NE	-7.36	96.35	111.80
1	B	412	ARG	CG-CD-NE	-6.85	97.41	111.80
1	B	355	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	412	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	B	375	ARG	CG-CD-NE	-5.91	99.39	111.80
1	B	412	ARG	CB-CA-C	-5.91	98.58	110.40
1	B	259	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	359	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	209	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	412	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	359	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	412	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	259	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3361	0	3270	16	0
1	B	3365	0	3263	12	0
2	A	53	0	29	0	0
2	B	53	0	29	0	0
3	A	6	0	8	0	0
3	B	12	0	16	0	0
4	A	5	0	10	1	0
5	A	6	0	11	1	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	B	10	0	19	0	0
8	A	274	0	0	4	0
8	B	244	0	0	1	0
All	All	7392	0	6655	28	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 2.

All (28) 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:67:ARG:NH1	1:B:441:GLN:OE1	2.04	0.91
1:A:432:TYR:CE1	4:A:503:13D:HCC1	2.15	0.82
1:A:400:PRO:HG3	8:A:805:HOH:O	1.89	0.71
1:B:9:VAL:HG11	1:B:248:VAL:HG21	1.81	0.61
1:A:22:ARG:NH2	1:A:74:GLU:OE1	2.30	0.58
1:A:187:HIS:HD2	8:A:840:HOH:O	1.90	0.54
1:A:150:GLU:OE1	8:A:601:HOH:O	2.18	0.54
1:B:187:HIS:HD2	8:B:806:HOH:O	1.91	0.54
1:B:6:VAL:O	1:B:257:ALA:HA	2.11	0.51
1:B:107:PHE:CZ	1:B:164:LEU:HD22	2.47	0.50
1:B:134:PRO:HG2	1:B:404:TRP:CE3	2.51	0.46
1:B:309:GLU:OE1	1:B:373:ARG:NH2	2.50	0.45
1:B:131:LEU:O	1:B:187:HIS:HE1	2.00	0.45
1:B:9:VAL:HG11	1:B:248:VAL:CG2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:VAL:O	1:B:256:ARG:HD2	2.17	0.43
1:A:267:THR:O	1:A:271:ARG:HG3	2.18	0.43
1:A:324:VAL:HG21	5:A:504:4HA:HE2	2.00	0.43
1:A:323:GLY:C	8:A:763:HOH:O	2.57	0.43
1:A:131:LEU:O	1:A:187:HIS:HE1	2.02	0.43
1:A:215:GLN:N	1:A:216:PRO:CD	2.82	0.42
1:A:134:PRO:HG2	1:A:404:TRP:CE3	2.54	0.42
1:B:322:ILE:HD11	1:B:342:PHE:CZ	2.55	0.41
1:A:248:VAL:O	1:A:254:GLU:HA	2.20	0.41
1:B:32:LEU:HD12	1:B:255:VAL:HG11	2.02	0.41
1:A:373:ARG:HG2	1:A:373:ARG:O	2.20	0.41
1:A:9:VAL:HG11	1:A:248:VAL:HG21	2.02	0.41
1:A:6:VAL:O	1:A:257:ALA:HA	2.20	0.40
1:A:394:CYS:CB	1:A:395:TYR:HA	2.52	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	448/474 (94%)	442 (99%)	6 (1%)	0	100	100
1	B	448/474 (94%)	441 (98%)	7 (2%)	0	100	100
All	All	896/948 (94%)	883 (98%)	13 (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	330/348 (95%)	327 (99%)	3 (1%)	75 72
1	B	330/348 (95%)	329 (100%)	1 (0%)	91 90
All	All	660/696 (95%)	656 (99%)	4 (1%)	84 82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	160	ARG
1	A	383	ARG
1	B	164	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
1	A	284	GLN
1	B	187	HIS
1	B	284	GLN
1	B	291	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 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	13D	A	503	-	4,4,4	0.35	0	3,3,3	0.43	0
5	4HA	A	504	-	5,5,5	1.87	1 (20%)	4,4,4	1.13	1 (25%)
2	FAD	A	501	1	53,58,58	1.49	9 (16%)	68,89,89	1.54	12 (17%)
3	GOL	B	503	-	5,5,5	0.20	0	5,5,5	0.48	0
3	GOL	A	502	-	5,5,5	0.25	0	5,5,5	0.75	0
2	FAD	B	501	1	53,58,58	1.17	4 (7%)	68,89,89	1.84	19 (27%)
3	GOL	B	504	-	5,5,5	0.11	0	5,5,5	0.40	0
7	SPD	B	502	-	9,9,9	0.12	0	8,8,8	0.42	0

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
4	13D	A	503	-	-	2/2/2/2	-
5	4HA	A	504	-	-	0/3/3/3	-
2	FAD	A	501	1	-	1/30/50/50	0/6/6/6
3	GOL	B	503	-	-	2/4/4/4	-
3	GOL	A	502	-	-	1/4/4/4	-
2	FAD	B	501	1	-	1/30/50/50	0/6/6/6
3	GOL	B	504	-	-	2/4/4/4	-
7	SPD	B	502	-	-	6/7/7/7	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C4X-N5	4.75	1.40	1.30
5	A	504	4HA	OA-CB	-4.17	1.20	1.42
2	B	501	FAD	C5'-C4'	3.81	1.57	1.51
2	A	501	FAD	O4B-C1B	3.14	1.45	1.41
2	A	501	FAD	C2B-C1B	-3.12	1.49	1.53
2	A	501	FAD	C1'-C2'	2.77	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C10-N1	2.53	1.38	1.33
2	A	501	FAD	C9-C9A	2.53	1.43	1.39
2	A	501	FAD	C7M-C7	2.46	1.55	1.51
2	A	501	FAD	O4-C4	2.44	1.28	1.23
2	A	501	FAD	C2A-N3A	2.35	1.35	1.32
2	A	501	FAD	C9A-C5X	-2.21	1.37	1.41
2	B	501	FAD	C4X-N5	2.16	1.34	1.30
2	B	501	FAD	O4-C4	2.02	1.27	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	FAD	N3A-C2A-N1A	-5.31	120.37	128.68
2	A	501	FAD	N3A-C2A-N1A	-4.73	121.29	128.68
2	B	501	FAD	C9A-C5X-N5	-4.15	117.93	122.43
2	B	501	FAD	C5'-C4'-C3'	-4.14	104.20	112.20
2	B	501	FAD	C4-N3-C2	-4.04	118.18	125.64
2	A	501	FAD	C4-N3-C2	-3.79	118.64	125.64
2	B	501	FAD	C10-C4X-N5	-3.55	117.31	124.86
2	A	501	FAD	C9A-N10-C10	-3.34	115.57	120.77
2	A	501	FAD	O3'-C3'-C4'	-3.22	101.02	108.81
2	B	501	FAD	O4B-C1B-C2B	-3.10	102.39	106.93
2	B	501	FAD	C8M-C8-C7	3.01	126.91	120.74
2	B	501	FAD	C4X-C10-N1	-2.76	118.32	124.73
2	A	501	FAD	O4-C4-C4X	-2.75	119.31	126.60
2	B	501	FAD	C4X-C4-N3	2.75	120.16	113.19
2	B	501	FAD	C5X-N5-C4X	2.74	122.64	118.07
2	A	501	FAD	C3B-C2B-C1B	2.61	104.91	100.98
2	B	501	FAD	C4-C4X-N5	2.60	121.94	118.23
2	B	501	FAD	O2P-P-O1P	2.48	124.51	112.24
2	B	501	FAD	C5X-C9A-N10	-2.48	115.40	117.95
2	A	501	FAD	C4X-C10-N10	2.44	120.05	116.48
2	A	501	FAD	O2P-P-O1P	2.44	124.31	112.24
2	B	501	FAD	C9-C9A-N10	2.42	125.11	121.84
2	A	501	FAD	C4X-C4-N3	2.29	119.00	113.19
5	A	504	4HA	OA-CB-CG	2.23	126.31	111.66
2	A	501	FAD	C9A-C5X-N5	-2.21	120.03	122.43
2	B	501	FAD	C3B-C2B-C1B	2.21	104.30	100.98
2	B	501	FAD	O4'-C4'-C3'	2.16	114.36	109.10
2	A	501	FAD	C10-C4X-N5	-2.15	120.29	124.86
2	A	501	FAD	P-O3P-PA	-2.12	125.55	132.83
2	B	501	FAD	C8M-C8-C9	-2.12	115.58	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	FAD	C1B-N9A-C4A	-2.07	123.00	126.64
2	B	501	FAD	C4X-C10-N10	2.05	119.48	116.48

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	504	GOL	C1-C2-C3-O3
7	B	502	SPD	N6-C7-C8-C9
3	B	503	GOL	C1-C2-C3-O3
3	B	504	GOL	O2-C2-C3-O3
7	B	502	SPD	C7-C8-C9-N10
3	A	502	GOL	C1-C2-C3-O3
3	B	503	GOL	O2-C2-C3-O3
7	B	502	SPD	C2-C3-C4-C5
7	B	502	SPD	C4-C5-N6-C7
4	A	503	13D	NAA-CA-CB-CC
2	B	501	FAD	O4B-C4B-C5B-O5B
4	A	503	13D	CA-CB-CC-ND
2	A	501	FAD	O4B-C4B-C5B-O5B
7	B	502	SPD	C8-C7-N6-C5
7	B	502	SPD	C3-C4-C5-N6

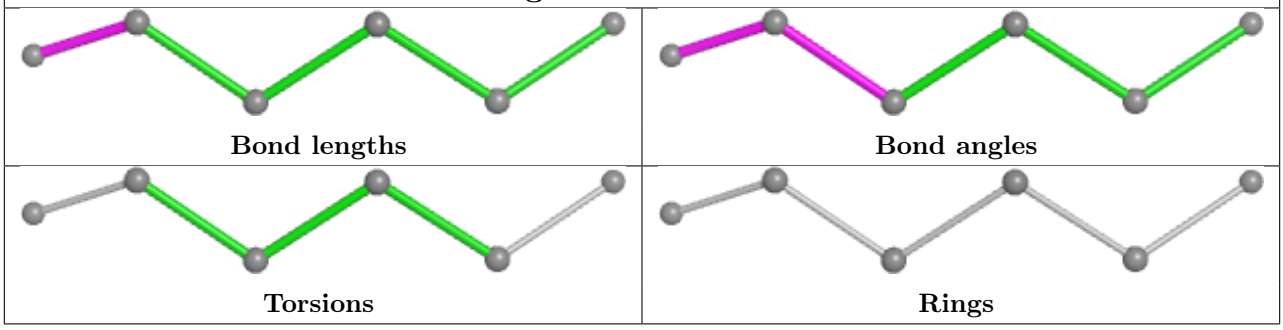
There are no ring outliers.

2 monomers are involved in 2 short contacts:

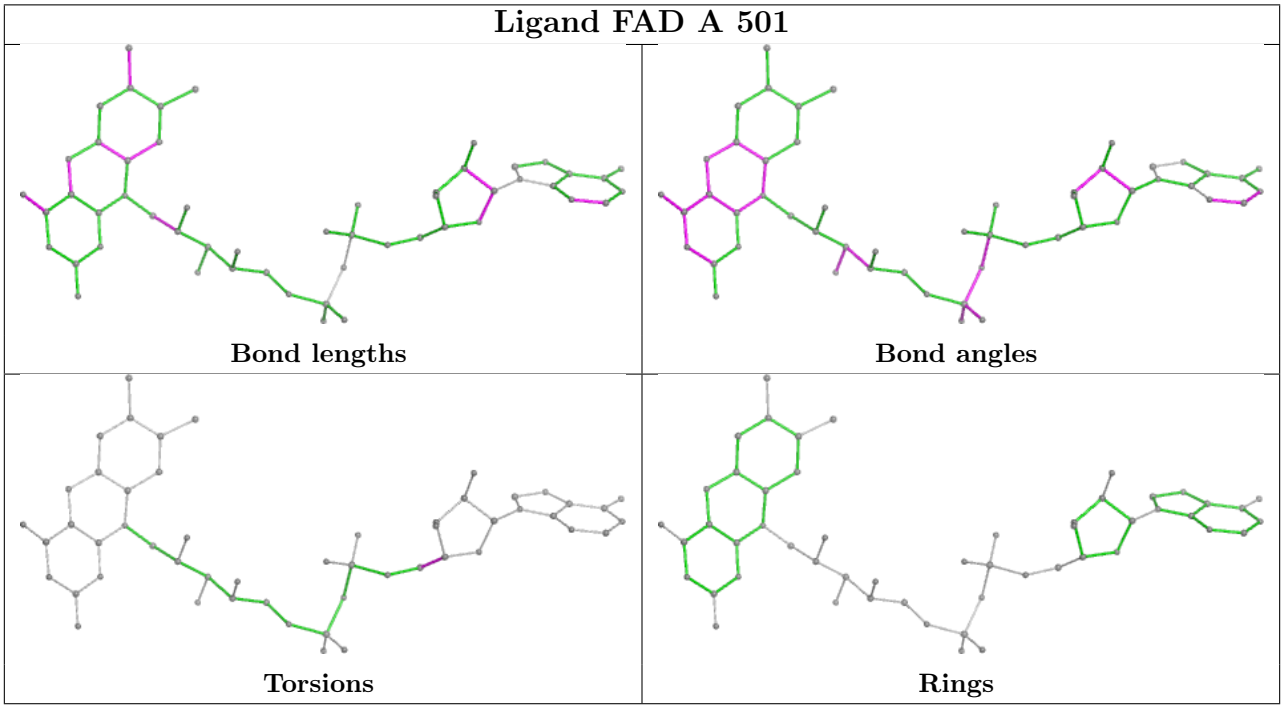
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	13D	1	0
5	A	504	4HA	1	0

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 then 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.

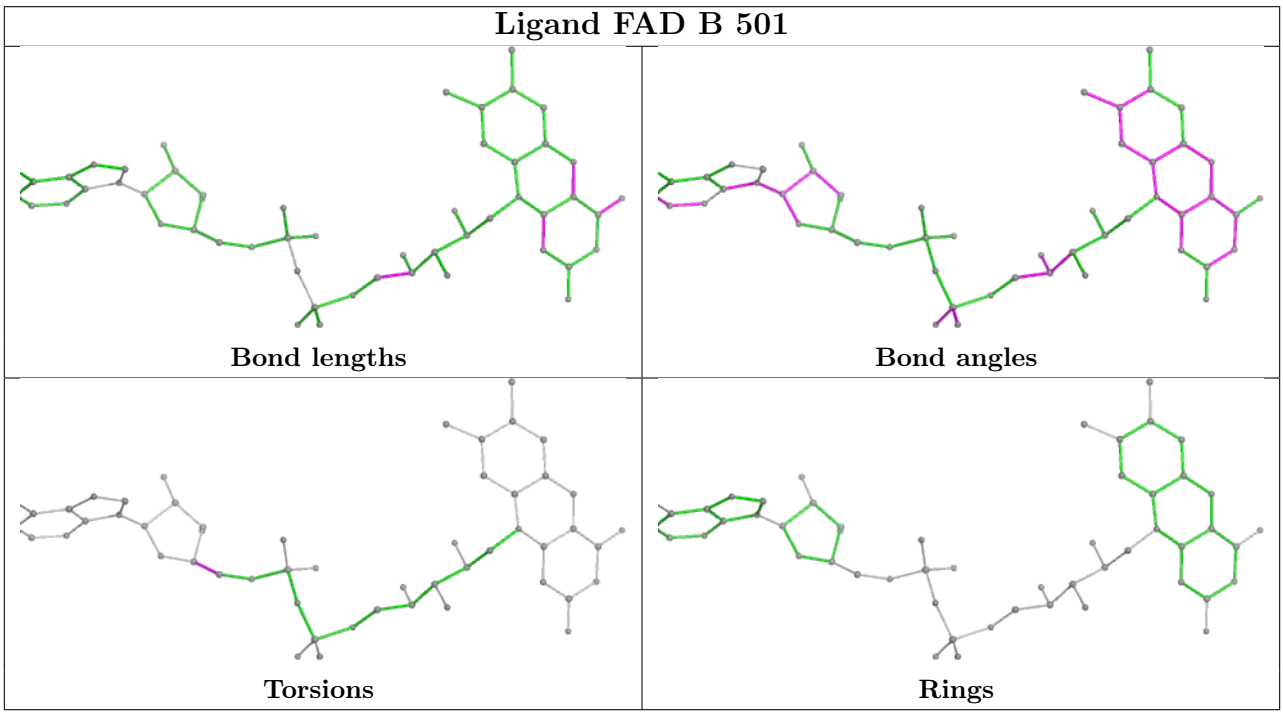
Ligand 4HA A 504

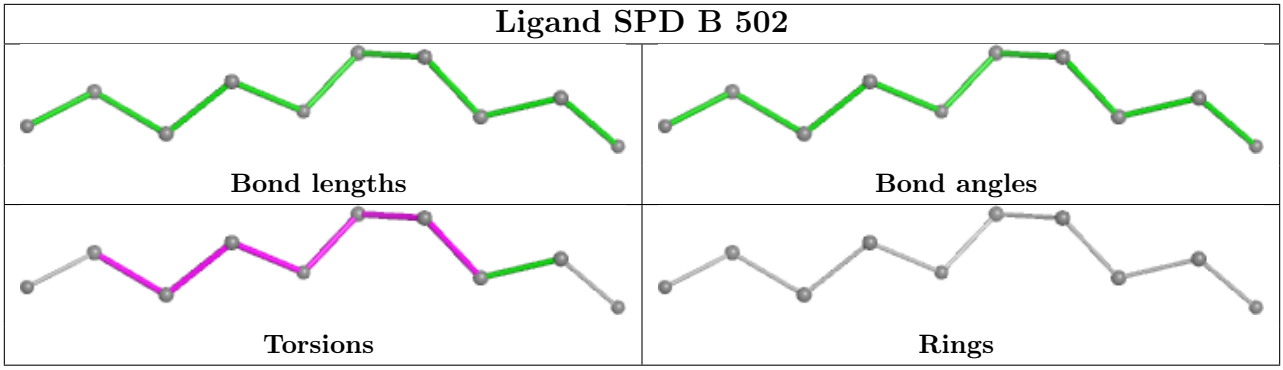


Ligand FAD A 501



Ligand FAD B 501





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	448/474 (94%)	-0.39	0 100 100	12, 20, 39, 54	2 (0%)
1	B	450/474 (94%)	-0.31	3 (0%) 84 84	15, 22, 38, 54	0
All	All	898/948 (94%)	-0.35	3 (0%) 90 90	12, 21, 38, 54	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	452	GLY	2.2
1	B	164	LEU	2.2
1	B	5	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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	GOL	B	504	6/6	0.83	0.14	28,38,40,45	0
5	4HA	A	504	6/6	0.87	0.18	50,51,51,54	0

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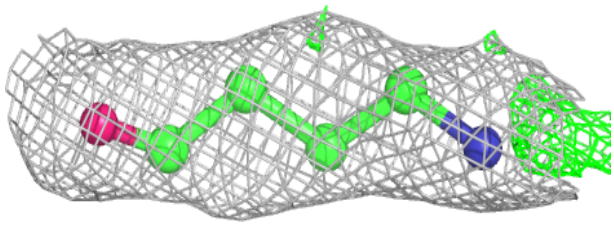
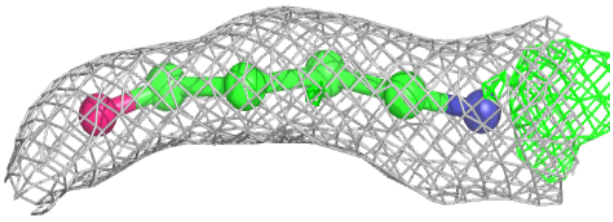
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SPD	B	502	10/10	0.88	0.14	40,48,51,51	0
4	13D	A	503	5/5	0.89	0.14	24,33,35,38	0
3	GOL	A	502	6/6	0.92	0.09	19,26,28,30	0
3	GOL	B	503	6/6	0.92	0.09	25,28,34,36	0
2	FAD	A	501	53/53	0.98	0.04	13,14,15,16	0
6	MG	B	505	1/1	0.98	0.05	28,28,28,28	0
2	FAD	B	501	53/53	0.98	0.04	14,16,18,18	0
6	MG	B	506	1/1	0.99	0.04	17,17,17,17	0
6	MG	A	505	1/1	0.99	0.03	31,31,31,31	0

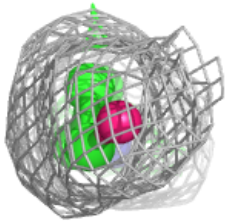
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4HA A 504:

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

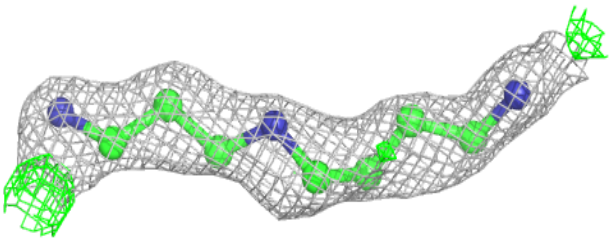


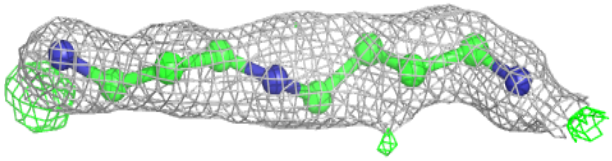


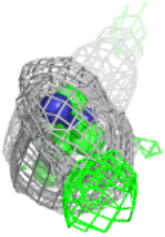


Electron density around SPD B 502:

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

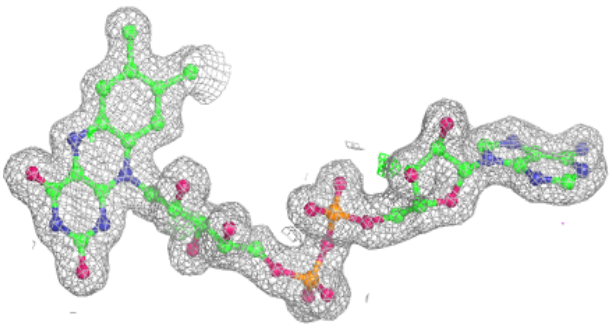


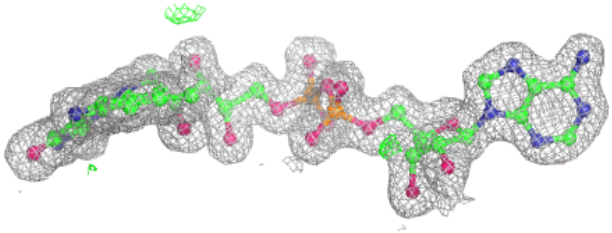


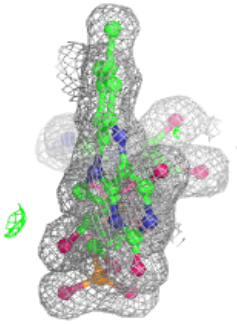


Electron density around FAD A 501:

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

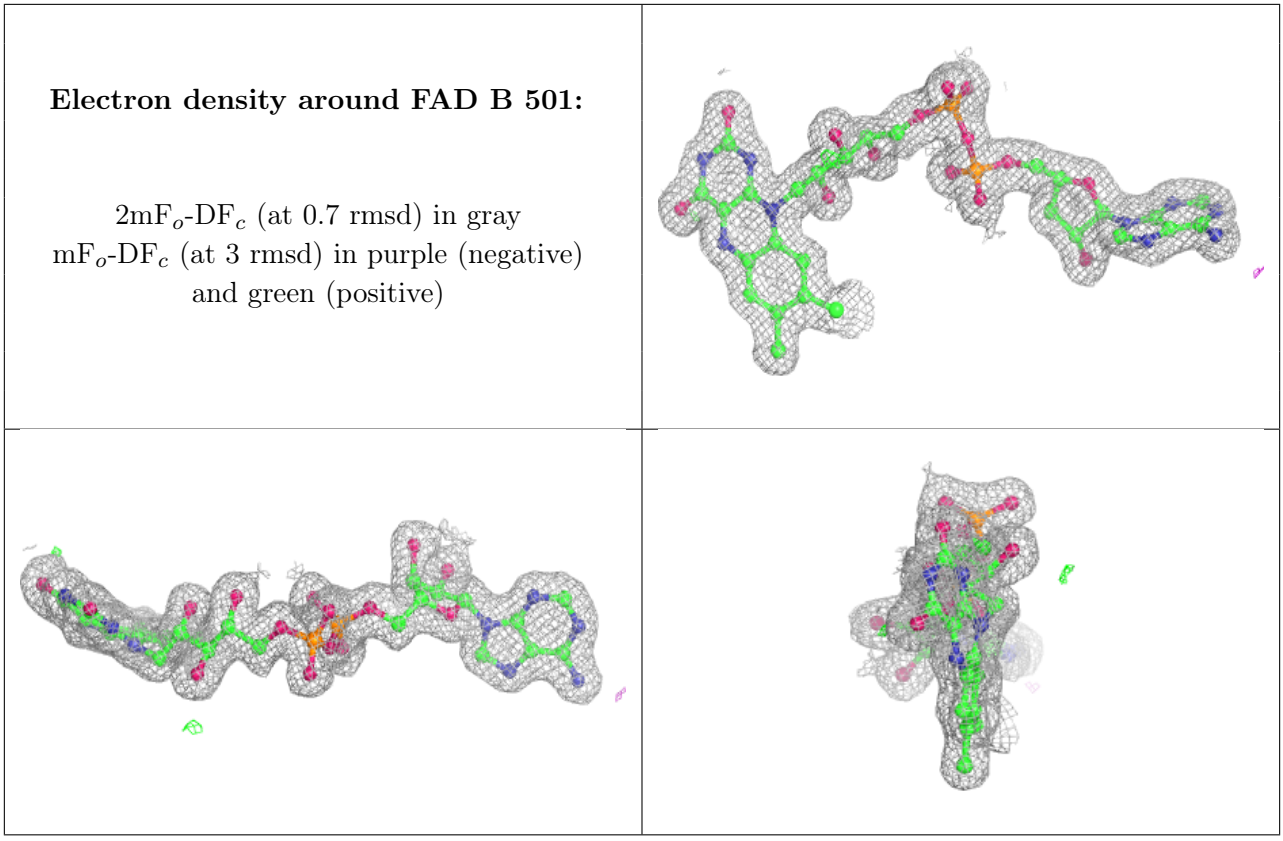






Electron density around FAD B 501:

$2mF_o$-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.