



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:10 pm BST

PDB ID : 1P4C
Title : High Resolution Structure of Oxidized Active Mutant of (S)-Mandelate Dehydrogenase
Authors : Sukumar, N.; Mitra, B.; Mathews, F.S.
Deposited on : 2003-04-22
Resolution : 1.35 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

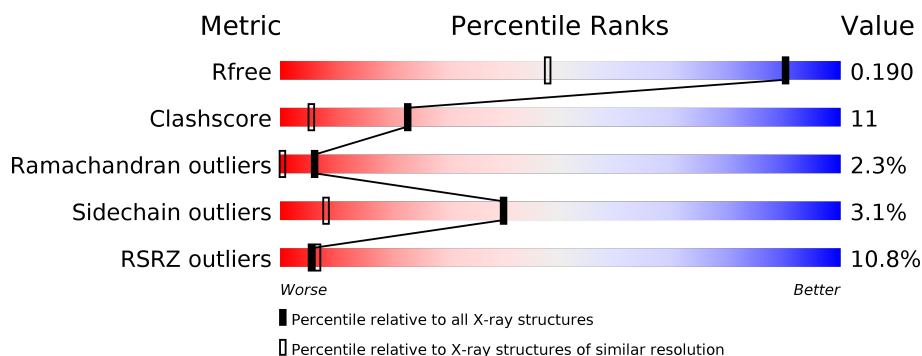
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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}	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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 on 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	380	<div> <div>10%</div> <div>78%</div> <div>12%</div> <div>7%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3195 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

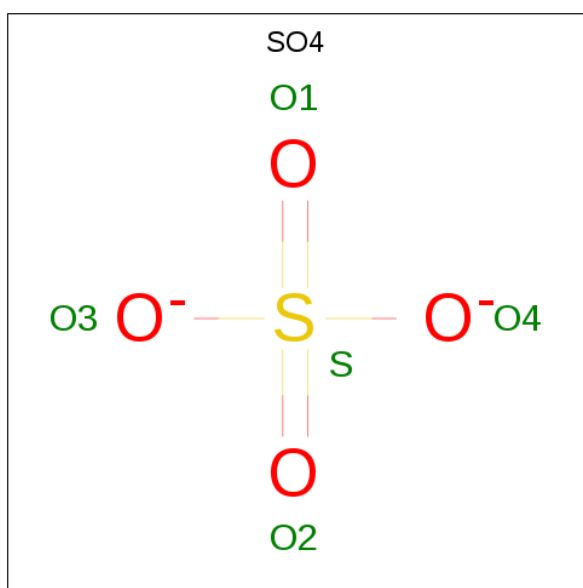
- Molecule 1 is a protein called L(+)-Mandelate Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	353	2747	1739	488	507	13	10	0	0

There are 7 discrepancies between the modelled and reference sequences:

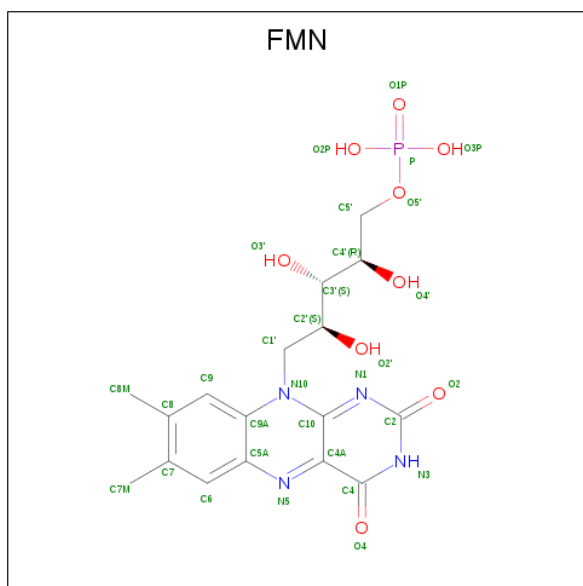
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ALA	ARG	SEE REMARK 999	UNP P20932
A	375	HIS	-	EXPRESSION TAG	UNP P20932
A	376	HIS	-	EXPRESSION TAG	UNP P20932
A	377	HIS	-	EXPRESSION TAG	UNP P20932
A	378	HIS	-	EXPRESSION TAG	UNP P20932
A	379	HIS	-	EXPRESSION TAG	UNP P20932
A	380	HIS	-	EXPRESSION TAG	UNP P20932

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



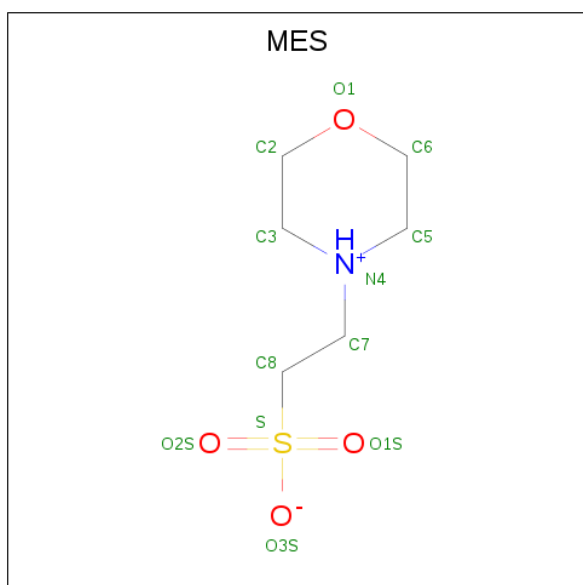
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

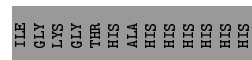


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	400	Total	O	0	0
			400	400		

- Molecule 1: L(+)-Mandelate Dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	99.40 Å 99.40 Å 87.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.60 – 1.35 39.60 – 1.35	Depositor EDS
% Data completeness (in resolution range)	96.5 (39.60-1.35) 96.6 (39.60-1.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 1.35 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.184 , 0.194 0.179 , 0.190	Depositor DCC
R_{free} test set	8965 reflections (9.68%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3195	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: FMN, SO4, MES

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	2/2796 (0.1%)	0.75	8/3782 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	LEU	N-CA	6.74	1.59	1.46
1	A	188	ASP	CB-CG	6.27	1.65	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ASN	N-CA-C	-8.93	86.90	111.00
1	A	193	ASP	CB-CG-OD1	8.15	125.64	118.30
1	A	193	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	189	LEU	N-CA-CB	6.92	124.25	110.40
1	A	189	LEU	CB-CG-CD1	6.35	121.80	111.00
1	A	188	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	190	GLY	N-CA-C	-6.07	97.91	113.10
1	A	194	LYS	C-N-CA	-5.89	106.98	121.70

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	2747	0	2781	64	0
2	A	5	0	0	0	0
3	A	31	0	19	1	0
4	A	12	0	13	0	0
5	A	400	0	0	2	0
All	All	3195	0	2813	64	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 11.

All (64) 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:189:LEU:HD12	1:A:190:GLY:H	1.16	1.08
1:A:63:GLN:OE1	1:A:70:ARG:HD2	1.66	0.94
1:A:192:MET:O	1:A:193:ASP:HB3	1.65	0.94
1:A:40:ASN:HD21	1:A:254:ASN:HD21	1.18	0.92
1:A:84:GLY:H	1:A:112:ASN:HD22	1.20	0.86
1:A:189:LEU:HD12	1:A:190:GLY:N	1.96	0.80
1:A:180:THR:OG1	1:A:182:LYS:HD3	1.82	0.79
1:A:195:ALA:O	1:A:196:ASN:HB2	1.84	0.77
1:A:192:MET:O	1:A:193:ASP:CB	2.33	0.76
1:A:189:LEU:HD13	1:A:200:GLN:NE2	2.01	0.74
1:A:196:ASN:O	1:A:197:LEU:HB2	1.94	0.68
1:A:193:ASP:O	1:A:194:LYS:C	2.35	0.65
1:A:189:LEU:CD1	1:A:190:GLY:H	2.03	0.64
1:A:137:ILE:HD13	1:A:203:LEU:HD21	1.79	0.63
1:A:195:ALA:O	1:A:196:ASN:CB	2.47	0.62
1:A:22:MET:CG	1:A:173:PHE:HD1	2.13	0.61
1:A:116:GLU:CD	1:A:116:GLU:H	2.04	0.60
1:A:187:ILE:HG22	1:A:187:ILE:O	2.01	0.60
1:A:193:ASP:O	1:A:197:LEU:HB2	2.03	0.59
1:A:84:GLY:H	1:A:112:ASN:ND2	1.96	0.58
1:A:159:VAL:HB	1:A:208:MET:HE1	1.86	0.58
1:A:135:ARG:HD2	5:A:1246:HOH:O	2.04	0.57
1:A:189:LEU:HD13	1:A:200:GLN:CD	2.25	0.57
1:A:116:GLU:OE2	1:A:144:LYS:HG2	2.05	0.57
1:A:40:ASN:ND2	1:A:254:ASN:HD21	1.97	0.57
1:A:133:ILE:N	1:A:133:ILE:HD12	2.21	0.56
1:A:85:ALA:N	1:A:179:LEU:HD11	2.20	0.56
1:A:189:LEU:HD13	1:A:200:GLN:HE22	1.70	0.55
1:A:200:GLN:HB3	1:A:204:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:HIS:HB3	1:A:137:ILE:HD12	1.92	0.52
1:A:186:GLY:O	1:A:188:ASP:N	2.39	0.52
1:A:284:ASP:O	1:A:285:SER:HB2	2.10	0.51
1:A:84:GLY:N	1:A:112:ASN:HD22	1.99	0.50
1:A:190:GLY:O	1:A:192:MET:SD	2.70	0.49
1:A:129:GLN:NE2	3:A:490:FMN:HN3	2.10	0.49
1:A:22:MET:HG3	1:A:173:PHE:HD1	1.77	0.48
1:A:134:HIS:CD2	1:A:136:GLU:HB3	2.49	0.48
1:A:85:ALA:HB2	1:A:179:LEU:HD11	1.96	0.47
1:A:320:THR:O	1:A:324:GLU:HG3	2.14	0.47
1:A:63:GLN:CD	1:A:70:ARG:HD2	2.32	0.47
1:A:193:ASP:O	1:A:194:LYS:O	2.32	0.47
1:A:147:HIS:HD2	5:A:1257:HOH:O	1.98	0.46
1:A:187:ILE:O	1:A:188:ASP:O	2.33	0.46
1:A:85:ALA:HB2	1:A:179:LEU:CD1	2.46	0.46
1:A:176:PRO:HB2	1:A:179:LEU:HG	1.99	0.44
1:A:131:TYR:CD1	1:A:208:MET:SD	3.10	0.44
1:A:112:ASN:HD21	1:A:179:LEU:HD13	1.81	0.44
1:A:112:ASN:HA	1:A:180:THR:O	2.18	0.44
1:A:200:GLN:HB3	1:A:204:MET:CE	2.47	0.44
1:A:75:LEU:HD21	1:A:293:ILE:HD13	2.00	0.44
1:A:176:PRO:O	1:A:179:LEU:HB2	2.18	0.43
1:A:59:ARG:HH11	1:A:59:ARG:HG3	1.84	0.42
1:A:197:LEU:HD12	1:A:200:GLN:NE2	2.33	0.42
1:A:116:GLU:CG	1:A:144:LYS:HE3	2.50	0.41
1:A:114:SER:HB2	1:A:116:GLU:OE1	2.19	0.41
1:A:177:PRO:C	1:A:179:LEU:H	2.23	0.41
1:A:284:ASP:O	1:A:285:SER:CB	2.69	0.41
1:A:108:SER:HA	1:A:129:GLN:HE21	1.86	0.41
1:A:137:ILE:CD1	1:A:203:LEU:HD11	2.51	0.41
1:A:134:HIS:HD2	1:A:137:ILE:HG13	1.86	0.40
1:A:203:LEU:C	1:A:205:SER:H	2.24	0.40
1:A:22:MET:CG	1:A:173:PHE:CD1	3.00	0.40
1:A:138:ALA:O	1:A:142:VAL:HG23	2.22	0.40
1:A:339:GLN:HB2	1:A:339:GLN:HE21	1.73	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	351/380 (92%)	332 (95%)	11 (3%)	8 (2%)	6 0

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ILE
1	A	188	ASP
1	A	194	LYS
1	A	197	LEU
1	A	189	LEU
1	A	193	ASP
1	A	196	ASN
1	A	285	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	288/311 (93%)	279 (97%)	9 (3%)	40 8

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	TYR
1	A	143	LEU
1	A	178	PHE

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Mol	Chain	Res	Type
1	A	179	LEU
1	A	180	THR
1	A	188	ASP
1	A	192	MET
1	A	207	GLN
1	A	310	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	40	ASN
1	A	46	GLN
1	A	112	ASN
1	A	121	GLN
1	A	129	GLN
1	A	134	HIS
1	A	147	HIS
1	A	162	ASN
1	A	200	GLN
1	A	272	GLN
1	A	339	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	FMN	A	490	-	31,33,33	3.80	12 (38%)	40,50,50	3.26	11 (27%)
4	MES	A	890	-	12,12,12	2.85	3 (25%)	14,16,16	1.08	0
2	SO4	A	901	-	4,4,4	0.47	0	6,6,6	0.07	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	MES	A	890	-	-	0/6/14/14	0/1/1/1
3	FMN	A	490	-	-	1/18/18/18	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	490	FMN	C4A-C10	14.59	1.53	1.38
4	A	890	MES	O1S-S	7.75	1.67	1.45
3	A	490	FMN	C9A-N10	6.30	1.47	1.38
3	A	490	FMN	C4-N3	6.01	1.43	1.33
3	A	490	FMN	C8-C7	5.16	1.53	1.40
3	A	490	FMN	C9A-C5A	5.05	1.52	1.42
3	A	490	FMN	C4-C4A	4.89	1.49	1.41
3	A	490	FMN	C2-N3	4.38	1.46	1.38
4	A	890	MES	O2S-S	4.23	1.57	1.45
3	A	490	FMN	C6-C7	3.69	1.47	1.37
3	A	490	FMN	C9-C9A	3.38	1.47	1.40
3	A	490	FMN	C5A-N5	2.80	1.40	1.35
4	A	890	MES	O3S-S	2.69	1.57	1.47
3	A	490	FMN	O2'-C2'	-2.67	1.37	1.43
3	A	490	FMN	O3'-C3'	2.14	1.48	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	490	FMN	C4-N3-C2	12.97	126.09	115.14
3	A	490	FMN	C4-C4A-C10	-8.60	114.26	119.95
3	A	490	FMN	C4A-C10-N10	-5.84	114.30	120.30
3	A	490	FMN	C4A-C4-N3	-5.77	115.54	123.43
3	A	490	FMN	C4A-N5-C5A	4.69	121.46	116.77
3	A	490	FMN	P-O5'-C5'	4.32	130.18	118.30
3	A	490	FMN	C5A-C9A-N10	-3.20	115.40	117.72
3	A	490	FMN	C10-C4A-N5	3.19	123.46	121.26
3	A	490	FMN	C4-C4A-N5	3.13	122.18	118.60
3	A	490	FMN	C5'-C4'-C3'	-2.30	107.77	112.20
3	A	490	FMN	O3'-C3'-C4'	-2.29	103.29	108.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

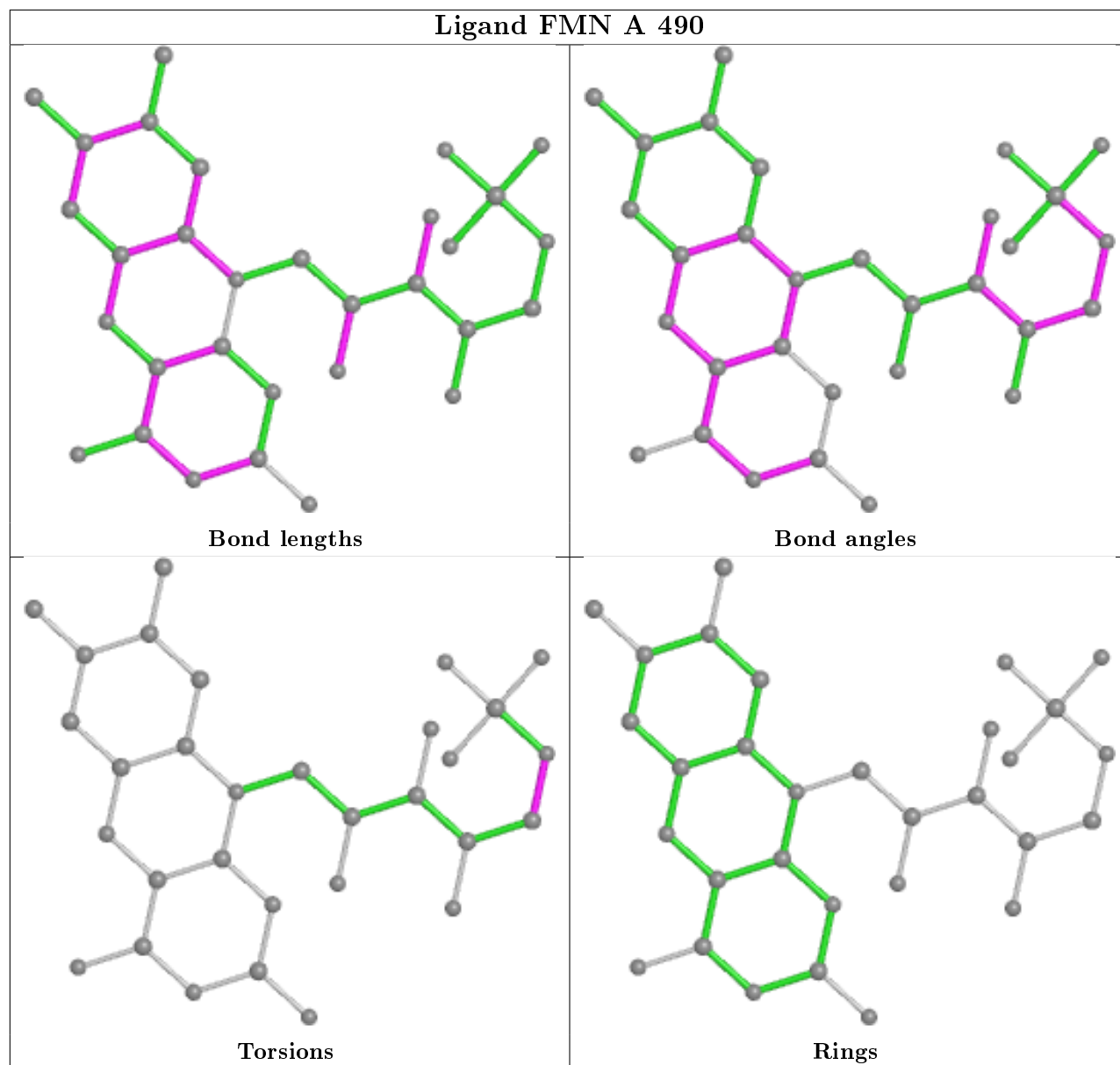
Mol	Chain	Res	Type	Atoms
3	A	490	FMN	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	490	FMN	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 ⓘ

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	353/380 (92%)	0.59	38 (10%) 5 7	11, 17, 53, 64	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	PHE	20.4
1	A	189	LEU	11.4
1	A	177	PRO	11.3
1	A	175	ILE	11.3
1	A	180	THR	10.3
1	A	187	ILE	9.4
1	A	176	PRO	9.3
1	A	179	LEU	8.8
1	A	190	GLY	8.6
1	A	186	GLY	7.3
1	A	204	MET	7.1
1	A	196	ASN	7.1
1	A	193	ASP	6.9
1	A	181	LEU	5.6
1	A	194	LYS	5.6
1	A	192	MET	5.5
1	A	4	ASN	5.4
1	A	188	ASP	4.9
1	A	174	LYS	4.5
1	A	197	LEU	4.4
1	A	203	LEU	4.1
1	A	207	GLN	3.5
1	A	205	SER	3.5
1	A	120	ARG	3.3
1	A	198	GLU	3.2
1	A	201	ALA	3.2
1	A	59	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	195	ALA	2.9
1	A	206	ARG	2.9
1	A	219	TRP	2.8
1	A	70	ARG	2.6
1	A	185	GLU	2.4
1	A	143	LEU	2.4
1	A	355	ASN	2.4
1	A	199	MET	2.3
1	A	136	GLU	2.3
1	A	305	LEU	2.2
1	A	304	VAL	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](#)

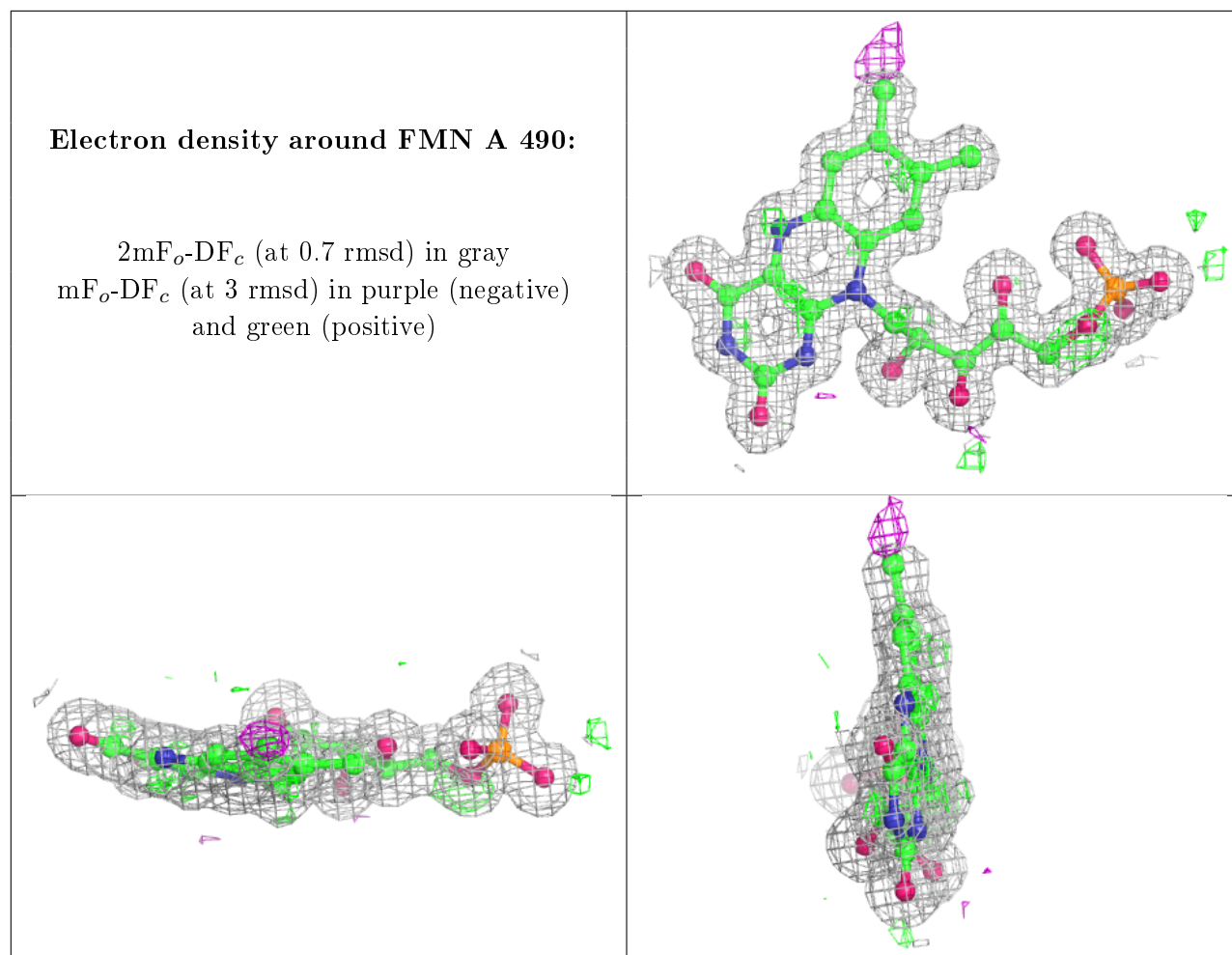
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
2	SO4	A	901	5/5	0.88	0.17	30,31,31,33	0
4	MES	A	890	12/12	0.97	0.07	14,16,19,22	0
3	FMN	A	490	31/31	0.98	0.10	11,13,15,16	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 ⓘ

There are no such residues in this entry.