



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:11 AM UTC

PDB ID : 8QNX / pdb_00008qnx
Title : OPR3 variant with redesigned loop 6 (8aa) in complex with NADH4
Authors : Bijelic, A.; Macheroux, P.; Kerschbaumer, B.
Deposited on : 2023-09-27
Resolution : 1.45 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

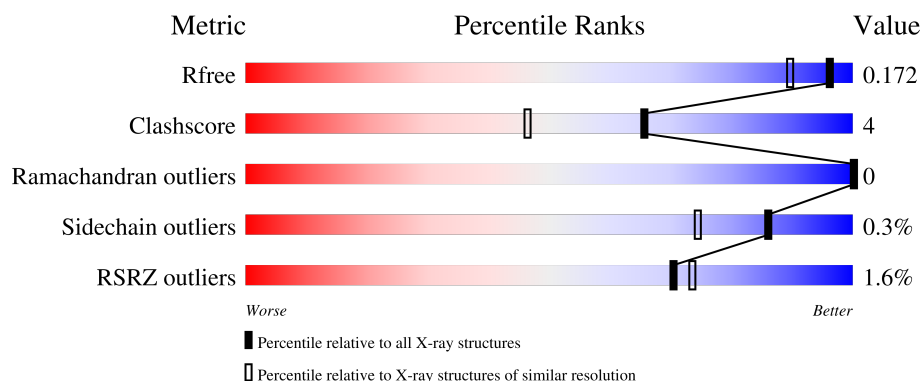
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

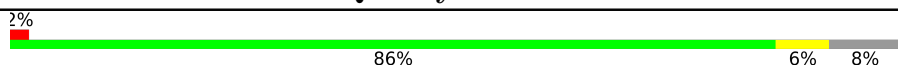
The reported resolution of this entry is 1.45 Å.

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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	396	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3389 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.

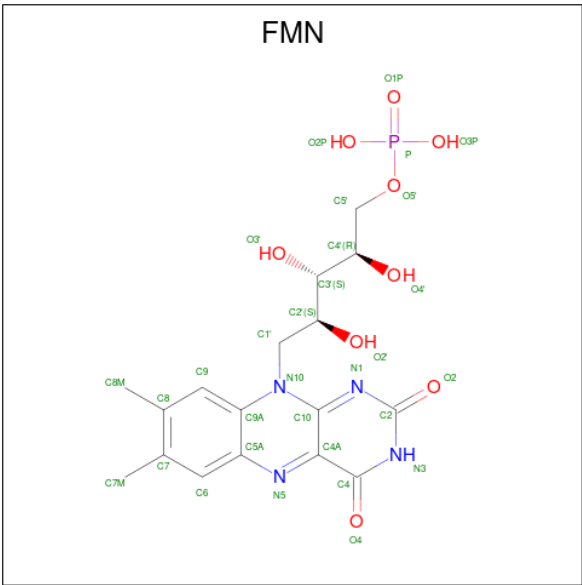
- Molecule 1 is a protein called 12-oxophytodienoate reductase 3.

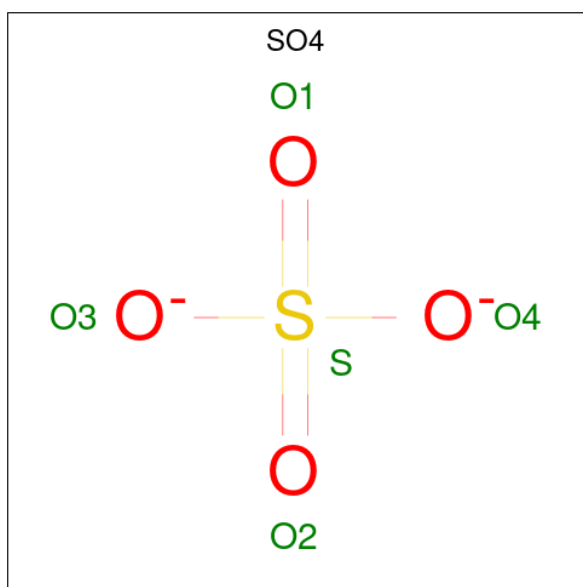
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	4	0
			2817	1791	506	509	11			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP Q9FEW9
A	-7	ALA	-	expression tag	UNP Q9FEW9
A	-6	SER	-	expression tag	UNP Q9FEW9
A	-5	HIS	-	expression tag	UNP Q9FEW9
A	-4	HIS	-	expression tag	UNP Q9FEW9
A	-3	HIS	-	expression tag	UNP Q9FEW9
A	-2	HIS	-	expression tag	UNP Q9FEW9
A	-1	HIS	-	expression tag	UNP Q9FEW9
A	0	HIS	-	expression tag	UNP Q9FEW9
A	283	GLY	ARG	engineered mutation	UNP Q9FEW9
A	284	ASP	TYR	engineered mutation	UNP Q9FEW9
A	285	GLY	VAL	engineered mutation	UNP Q9FEW9
A	286	ARG	ALA	engineered mutation	UNP Q9FEW9
A	?	-	TYR	deletion	UNP Q9FEW9
A	?	-	GLY	deletion	UNP Q9FEW9
A	?	-	GLN	deletion	UNP Q9FEW9
A	?	-	THR	deletion	UNP Q9FEW9
A	?	-	GLU	deletion	UNP Q9FEW9
A	?	-	ALA	deletion	UNP Q9FEW9
A	?	-	GLY	deletion	UNP Q9FEW9
A	?	-	ARG	deletion	UNP Q9FEW9
A	?	-	LEU	deletion	UNP Q9FEW9

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).





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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	466	Total	O	0	0
			466	466		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.01Å 89.62Å 49.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.01 – 1.45 44.01 – 1.45	Depositor EDS
% Data completeness (in resolution range)	93.4 (44.01-1.45) 93.4 (44.01-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 1.45Å)	Xtriage
Refinement program	PHENIX (dev_4761: ???)	Depositor
R, R_{free}	0.147 , 0.172 0.148 , 0.172	Depositor DCC
R_{free} test set	3269 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3389	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SO4, WI6

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	0.71	0/2895	0.83	0/3933

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	ARG	Sidechain

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	2817	0	2786	22	0
2	A	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	70	0	0	0	0
4	A	5	0	0	0	0
5	A	466	0	0	11	0
All	All	3389	0	2805	22	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 4.

All (22) 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:251[B]:ASN:ND2	5:A:501:HOH:O	2.06	0.89
1:A:261:GLU:OE1	5:A:502:HOH:O	2.09	0.70
1:A:261:GLU:OE1	5:A:503:HOH:O	2.13	0.67
1:A:232:ASP:OD1	5:A:504:HOH:O	2.17	0.58
1:A:135:ASN:HB2	1:A:138:ARG:HH12	1.68	0.57
1:A:261:GLU:CD	1:A:265:LYS:NZ	2.62	0.57
1:A:251[B]:ASN:ND2	5:A:506:HOH:O	2.37	0.57
1:A:265:LYS:HG2	5:A:687:HOH:O	2.06	0.54
1:A:162:GLN:HG2	5:A:837:HOH:O	2.12	0.49
1:A:261:GLU:OE2	1:A:265:LYS:NZ	2.46	0.49
1:A:66:MET:HB2	1:A:79:GLY:HA2	1.94	0.49
1:A:261:GLU:CD	1:A:265:LYS:HZ3	2.23	0.45
1:A:241:ALA:HB3	5:A:898:HOH:O	2.17	0.44
1:A:90:LYS:HD2	5:A:558:HOH:O	2.19	0.42
1:A:168:ARG:HD2	5:A:744:HOH:O	2.19	0.42
1:A:19:GLY:HA3	5:A:665:HOH:O	2.19	0.42
1:A:297[A]:ARG:HD3	1:A:326:ASP:OD1	2.20	0.42
1:A:114:SER:HB3	1:A:125:PRO:HB3	2.02	0.42
1:A:182:ILE:C	1:A:182:ILE:HD12	2.45	0.42
1:A:112:ARG:HB3	1:A:127:SER:HB2	2.03	0.41
1:A:334:ARG:HB3	1:A:355:TYR:CE2	2.56	0.40
1:A:344:MET:HE2	1:A:344:MET:HA	2.04	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	364/396 (92%)	355 (98%)	9 (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	293/323 (91%)	292 (100%)	1 (0%)	86	74

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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
3	WI6	A	402[B]	-	47,48,48	0.57	0	66,73,73	0.73	2 (3%)
3	WI6	A	402[A]	-	25,27,48	2.03	5 (20%)	35,41,73	1.82	8 (22%)
4	SO4	A	403	-	4,4,4	0.35	0	6,6,6	0.07	0
2	FMN	A	401	-	33,33,33	1.37	3 (9%)	48,50,50	1.11	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	WI6	A	402[B]	-	-	8/30/72/72	0/5/5/5
3	WI6	A	402[A]	-	-	9/20/46/72	0/2/2/5
2	FMN	A	401	-	-	1/18/18/18	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[A]	WI6	PN-O3	8.25	1.68	1.59
2	A	401	FMN	C4A-N5	3.92	1.39	1.30
2	A	401	FMN	C6-C7	-3.57	1.34	1.39
3	A	402[A]	WI6	O7N-C7N	-2.66	1.19	1.23
3	A	402[A]	WI6	PA-O5'	2.61	1.64	1.54
3	A	402[A]	WI6	C2N-N1N	-2.56	1.43	1.47
2	A	401	FMN	C1'-C2'	2.54	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[A]	WI6	PN-O5'A	2.06	1.67	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402[A]	WI6	C6N-N1N-C2N	5.15	117.35	109.43
3	A	402[A]	WI6	C3N-C4N-C5N	-4.13	116.31	123.33
3	A	402[A]	WI6	C4N-C3N-C7N	4.03	121.11	109.80
3	A	402[B]	WI6	C6N-N1N-C2N	3.46	114.75	109.43
3	A	402[B]	WI6	C3N-C4N-C5N	-3.05	118.13	123.33
3	A	402[A]	WI6	O4'A-C4'A-C5'A	2.83	118.39	109.33
3	A	402[A]	WI6	O5'-PA-O3	-2.59	95.95	104.64
2	A	401	FMN	C10-C4A-N5	-2.52	119.66	124.81
3	A	402[A]	WI6	C6N-N1N-C1'A	2.47	120.10	112.93
2	A	401	FMN	C5A-C9A-N10	2.41	120.15	117.97
2	A	401	FMN	C4A-C10-N10	2.36	119.87	116.48
3	A	402[A]	WI6	C5'A-C4'A-C3'A	-2.02	107.95	115.21
3	A	402[A]	WI6	O1-PA-O2P	2.00	118.63	110.83

There are no chirality outliers.

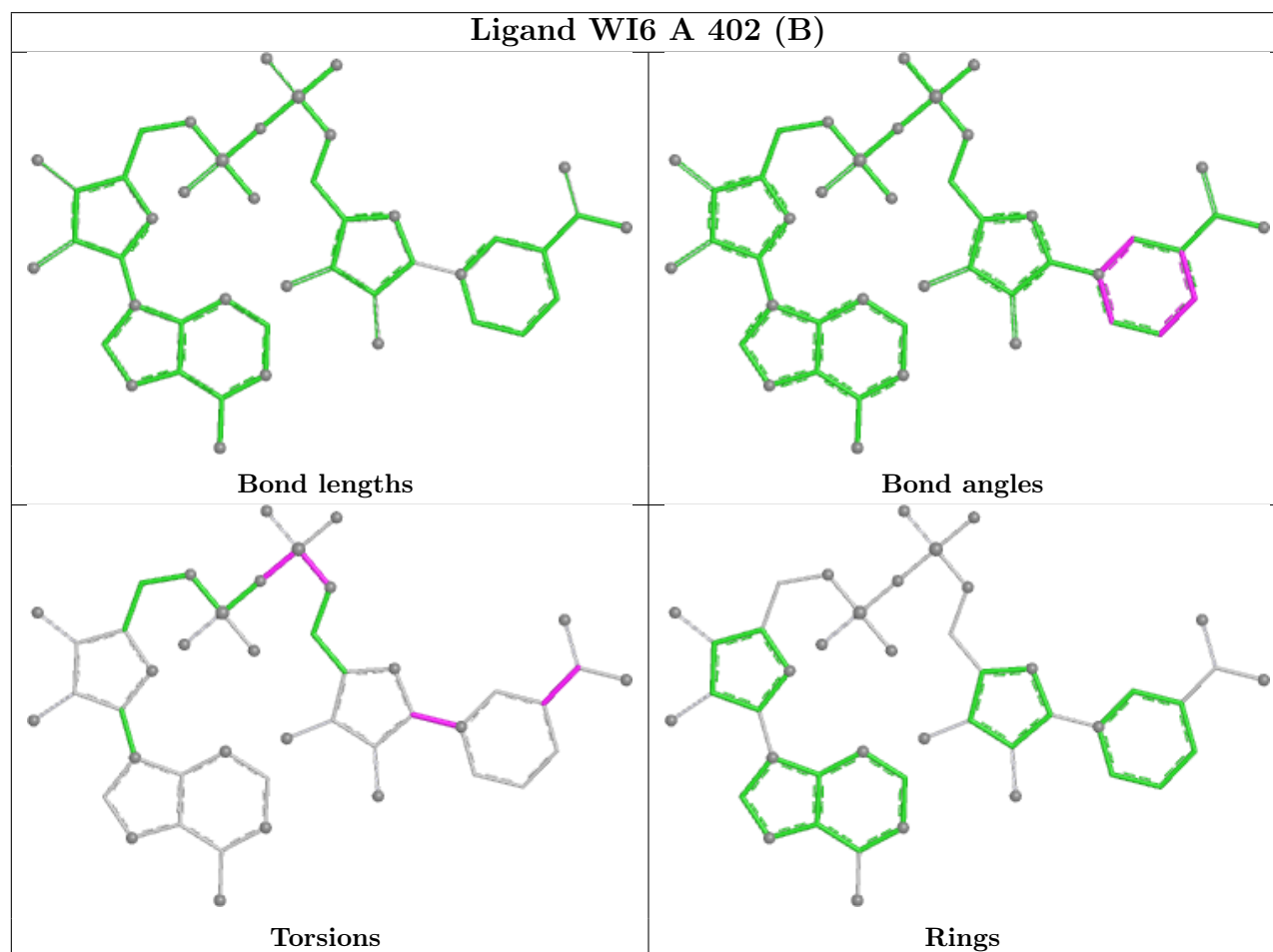
All (18) torsion outliers are listed below:

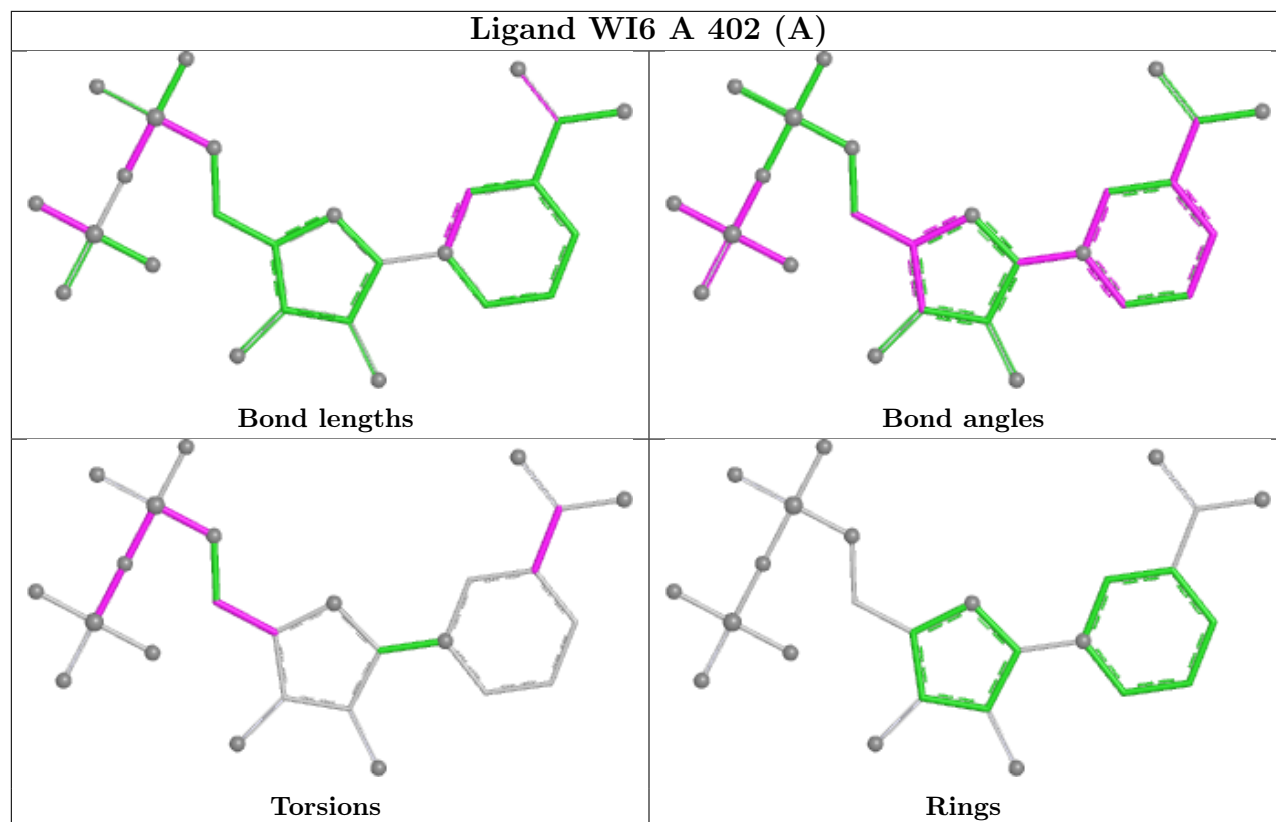
Mol	Chain	Res	Type	Atoms
3	A	402[A]	WI6	C4N-C3N-C7N-N7N
3	A	402[A]	WI6	C5'A-O5'A-PN-O1N
3	A	402[A]	WI6	C5'A-O5'A-PN-O2N
3	A	402[A]	WI6	C5'A-O5'A-PN-O3
3	A	402[B]	WI6	O4'A-C1'A-N1N-C2N
3	A	402[B]	WI6	C5'A-O5'A-PN-O2N
3	A	402[B]	WI6	C5'A-O5'A-PN-O3
3	A	402[A]	WI6	O4'A-C4'A-C5'A-O5'A
3	A	402[A]	WI6	C3'A-C4'A-C5'A-O5'A
3	A	402[B]	WI6	C2N-C3N-C7N-N7N
3	A	402[B]	WI6	C2N-C3N-C7N-O7N
3	A	402[B]	WI6	PA-O3-PN-O5'A
3	A	402[A]	WI6	PN-O3-PA-O2P
3	A	402[A]	WI6	PA-O3-PN-O2N
2	A	401	FMN	C4'-C5'-O5'-P
3	A	402[B]	WI6	C2'A-C1'A-N1N-C2N
3	A	402[A]	WI6	PA-O3-PN-O1N
3	A	402[B]	WI6	PA-O3-PN-O2N

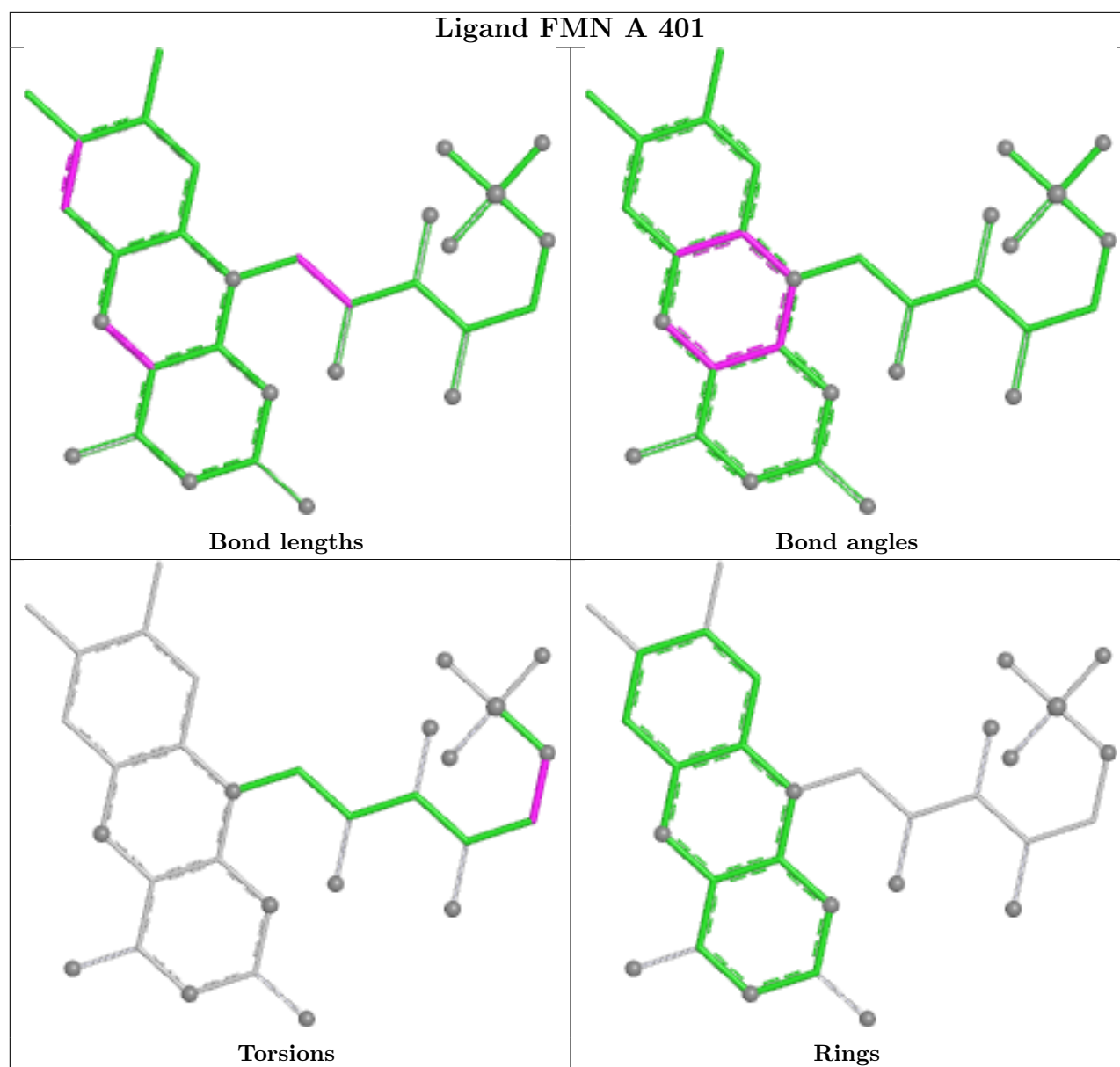
There are no ring outliers.

No monomer is involved in short contacts.

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	364/396 (91%)	-0.32	6 (1%) 70 73	10, 14, 28, 49	4 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	ASP	4.1
1	A	288	SER	3.3
1	A	285	GLY	2.9
1	A	292	GLU	2.4
1	A	269[A]	HIS	2.3
1	A	248	MET	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(Å ²)	Q<0.9
4	SO4	A	403	5/5	0.67	0.12	41,44,71,94	0

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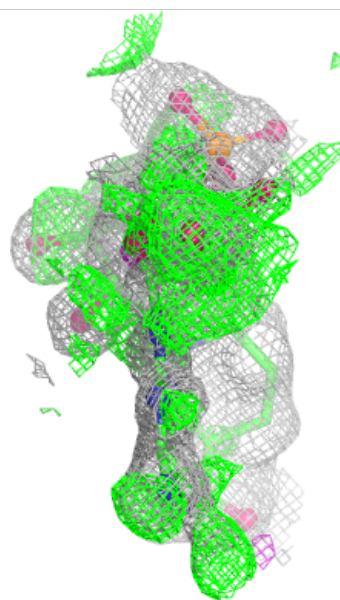
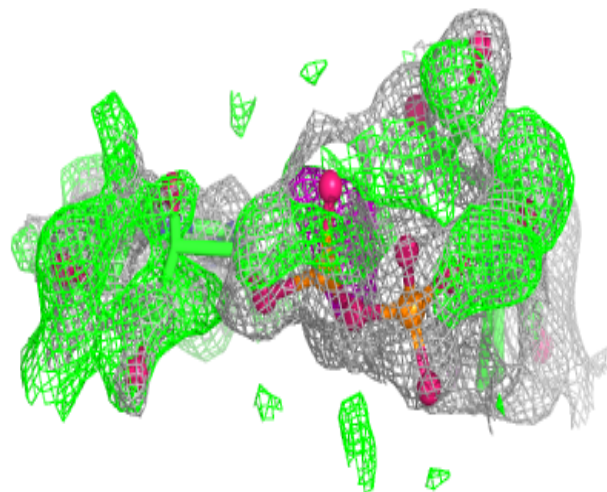
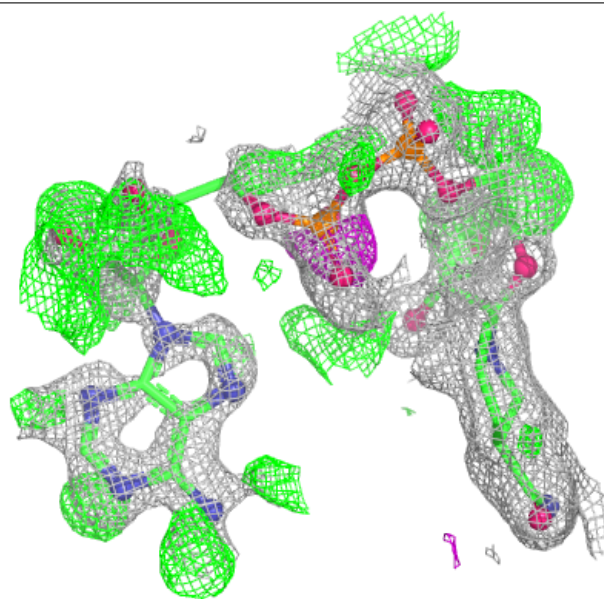
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	WI6	A	402[B]	44/44	0.73	0.19	9,24,30,36	44
3	WI6	A	402[A]	26/44	0.73	0.19	7,20,46,52	26
2	FMN	A	401	31/31	0.98	0.04	9,10,13,18	0

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.

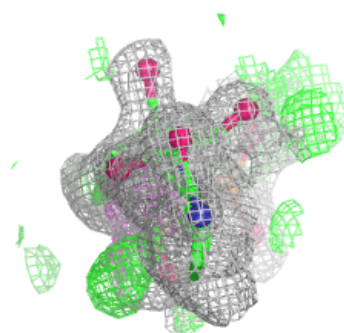
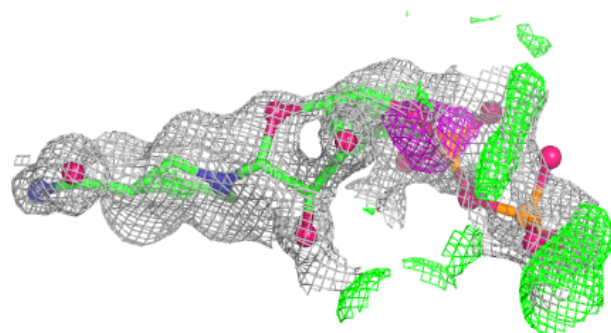
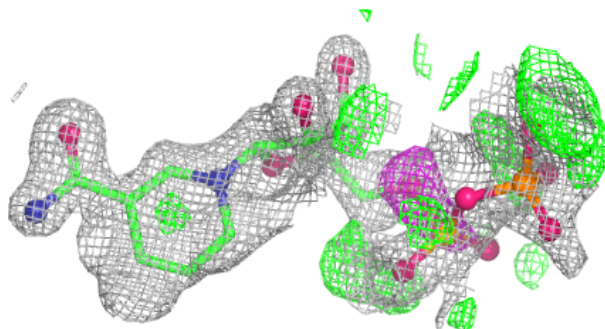
Electron density around WI6 A 402 (B):

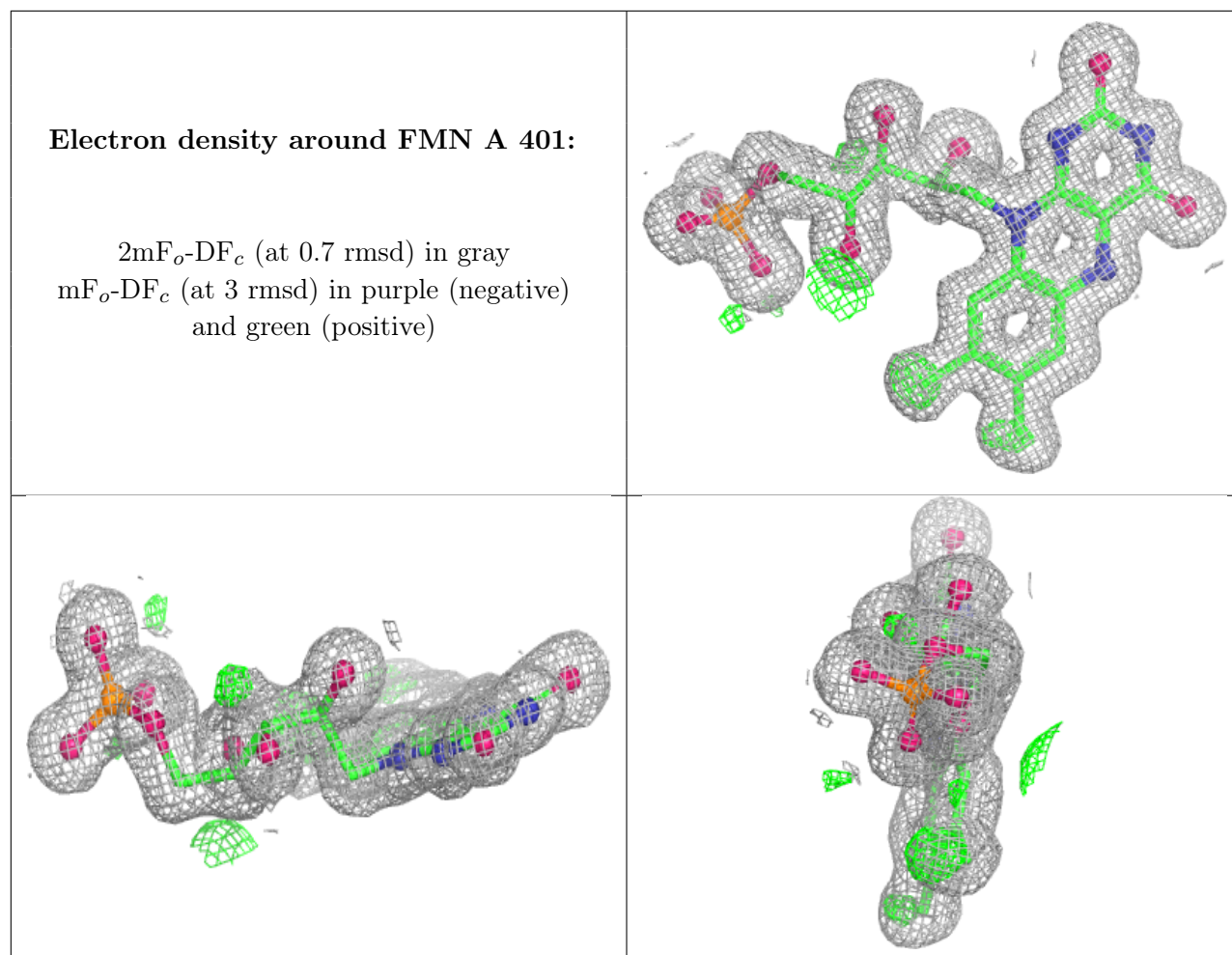
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around WI6 A 402 (A):

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





6.5 Other polymers ⓘ

There are no such residues in this entry.