Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 09:36 am BST

PDB ID	:	4AEO
Title	:	Structure of Xenobiotic Reductase B from Pseudomonas putida in complex with TNT
Authors	:	Carvalho, A.L.; Mukhopadhyay, A.; Romao, M.J.; Bursakov, S.; Kladova, A.; Ramos, J.L.; van Dillewijn, P.
Deposited on	:	2012-01-11
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

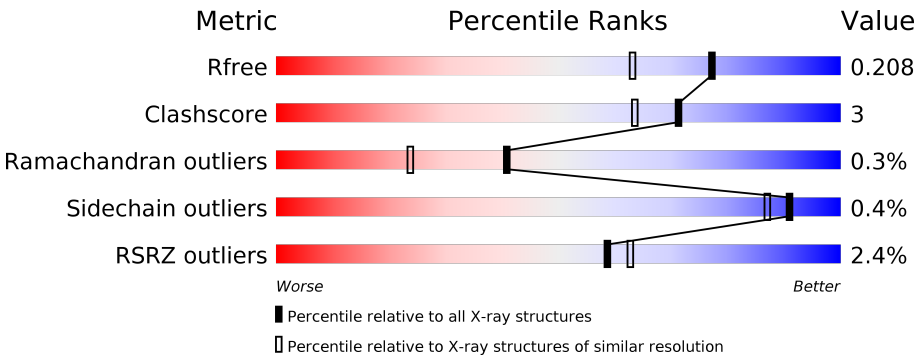
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 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 <=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	362	2% 91% 6% •
1	B	362	3% 90% 7% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TNL	A	1355	-	-	X	X
5	TNL	B	1353	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6953 atoms, of which 740 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 XENOBIOTIC REDUCTASE B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	349	3017	1677	353	475	506	6	0	4	0
1	B	349	3025	1682	353	473	511	6	0	4	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	LYS	-	expression tag	UNP Q88PD0
A	351	LEU	-	expression tag	UNP Q88PD0
A	352	ALA	-	expression tag	UNP Q88PD0
A	353	ALA	-	expression tag	UNP Q88PD0
A	354	ALA	-	expression tag	UNP Q88PD0
A	355	LEU	-	expression tag	UNP Q88PD0
A	356	GLU	-	expression tag	UNP Q88PD0
A	357	HIS	-	expression tag	UNP Q88PD0
A	358	HIS	-	expression tag	UNP Q88PD0
A	359	HIS	-	expression tag	UNP Q88PD0
A	360	HIS	-	expression tag	UNP Q88PD0
A	361	HIS	-	expression tag	UNP Q88PD0
A	362	HIS	-	expression tag	UNP Q88PD0
B	350	LYS	-	expression tag	UNP Q88PD0
B	351	LEU	-	expression tag	UNP Q88PD0
B	352	ALA	-	expression tag	UNP Q88PD0
B	353	ALA	-	expression tag	UNP Q88PD0
B	354	ALA	-	expression tag	UNP Q88PD0
B	355	LEU	-	expression tag	UNP Q88PD0
B	356	GLU	-	expression tag	UNP Q88PD0
B	357	HIS	-	expression tag	UNP Q88PD0
B	358	HIS	-	expression tag	UNP Q88PD0
B	359	HIS	-	expression tag	UNP Q88PD0
B	360	HIS	-	expression tag	UNP Q88PD0
B	361	HIS	-	expression tag	UNP Q88PD0

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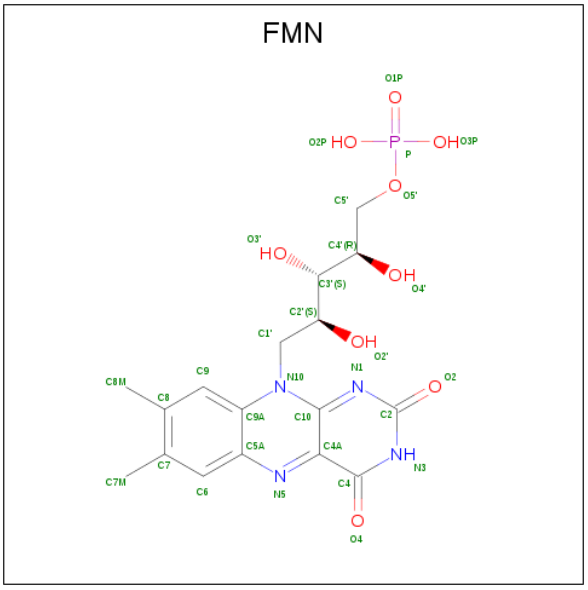
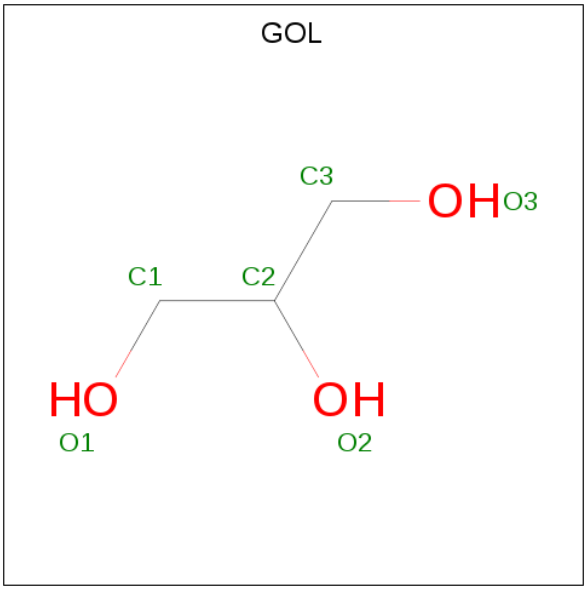
Chain	Residue	Modelled	Actual	Comment	Reference
B	362	HIS	-	expression tag	UNP Q88PD0

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



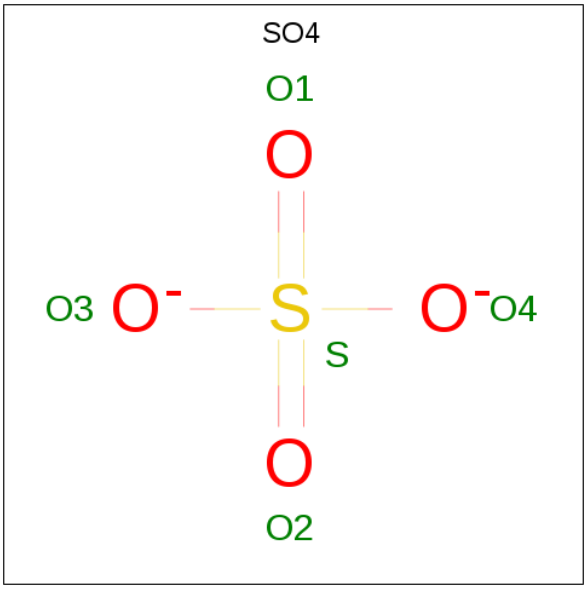
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	39	17	8	4	9	1	0	0
			Total	C	H	N	O	P		
2	B	1	39	17	8	4	9	1	0	0

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



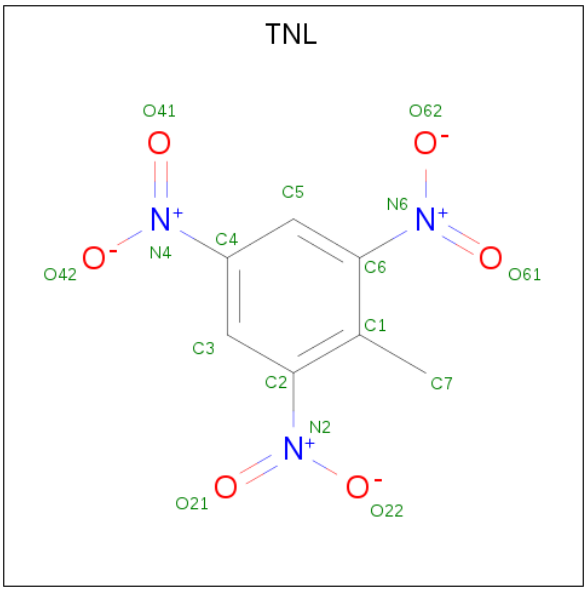
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	14	3	8	3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is 2,4,6-TRINITROTOLUENE (three-letter code: TNL) (formula: $C_7H_5N_3O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
5	A	1	21	7	5	3	6	0	0
			Total	C	H	N	O		
5	B	1	21	7	5	3	6	0	0

- Molecule 6 is water.

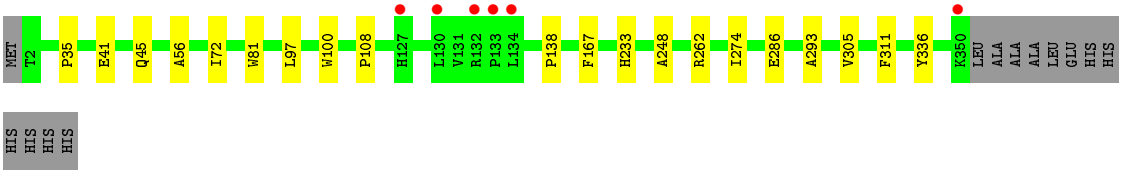
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	417	417	417	0	0
			Total	O		
6	B	345	345	345	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

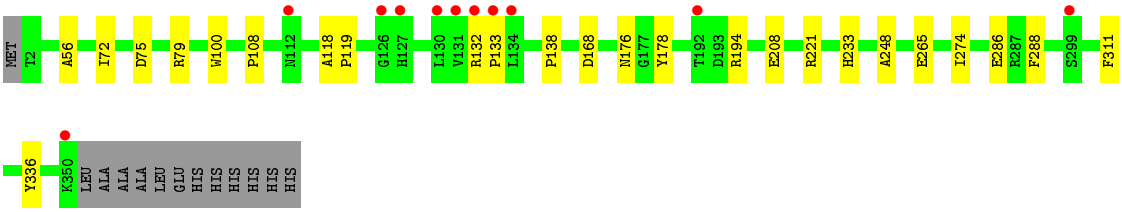
- Molecule 1: XENOBIOTIC REDUCTASE B

Chain A:



- Molecule 1: XENOBIOTIC REDUCTASE B

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	67.18Å 105.32Å 106.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.57 – 1.70 25.56 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (25.57-1.70) 95.2 (25.56-1.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 1.70Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.172 , 0.205 0.172 , 0.208	Depositor DCC
R_{free} test set	8020 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å^2)	11.4	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.035 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6953	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3343e-03.*

[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 (i)

5.1 Standard geometry (i)

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

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	0.38	0/2739	0.56	0/3733
1	B	0.38	0/2747	0.55	0/3743
All	All	0.38	0/5486	0.55	0/7476

There are no bond length outliers.

There are no bond angle outliers.

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	2664	353	2588	13	0
1	B	2672	353	2595	16	0
2	A	31	8	19	4	0
2	B	31	8	19	4	0
3	A	6	8	8	0	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
5	A	16	5	5	8	0
5	B	16	5	5	8	0
6	A	417	0	0	0	0
6	B	345	0	0	1	0
All	All	6213	740	5239	37	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 3.

All (37) 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:262:ARG:HD3	5:A:1355:TNL:O62	1.80	0.82
1:B:233:HIS:CE1	5:B:1353:TNL:O21	2.40	0.74
2:B:1351:FMN:N3	5:B:1353:TNL:O41	2.21	0.73
2:B:1351:FMN:C2	5:B:1353:TNL:O41	2.40	0.69
1:A:262:ARG:CD	5:A:1355:TNL:O62	2.46	0.64
2:A:1351:FMN:H1'1	5:A:1355:TNL:O62	2.01	0.60
2:B:1351:FMN:C4	5:B:1353:TNL:O41	2.52	0.57
1:A:233:HIS:HE1	5:A:1355:TNL:H3	1.71	0.56
1:B:56:ALA:HB1	1:B:100:TRP:CD2	2.41	0.56
1:A:72:ILE:O	1:A:72:ILE:HG13	2.05	0.55
1:B:176:ASN:HB2	5:B:1353:TNL:O42	2.07	0.55
2:A:1351:FMN:C1'	5:A:1355:TNL:O62	2.55	0.55
5:A:1355:TNL:H7C1	5:A:1355:TNL:O61	2.08	0.54
1:B:118:ALA:HB1	1:B:119:PRO:HD2	1.89	0.53
1:A:56:ALA:HB1	1:A:100:TRP:CD2	2.45	0.52
1:B:72:ILE:HG13	1:B:72:ILE:O	2.10	0.51
1:B:194:ARG:NH2	1:B:208:GLU:OE2	2.43	0.51
1:B:176:ASN:HB3	5:B:1353:TNL:H3	1.93	0.50
1:A:248:ALA:HB2	1:A:274:ILE:HG23	1.94	0.49
1:A:293:ALA:HB1	1:A:305:VAL:HG21	1.95	0.48
1:A:108:PRO:HD3	1:A:138:PRO:HG3	1.95	0.48
1:B:168:ASP:O	1:B:221:ARG:HD2	2.15	0.47
1:A:97:LEU:HD13	1:A:167:PHE:CZ	2.48	0.47
1:A:233:HIS:CE1	5:A:1355:TNL:H3	2.51	0.46
1:B:178:TYR:HE2	5:B:1353:TNL:O42	1.98	0.46
1:B:132:ARG:HA	1:B:133:PRO:C	2.35	0.45
1:A:41:GLU:O	1:A:45:GLN:HG3	2.16	0.45
1:B:108:PRO:HD3	1:B:138:PRO:HG3	1.99	0.45
1:B:75[B]:ASP:OD2	1:B:79:ARG:NH1	2.50	0.45
2:A:1351:FMN:H1'2	5:A:1355:TNL:N6	2.32	0.44
1:A:35:PRO:HG2	1:A:81:TRP:CG	2.52	0.44
1:B:265[A]:GLU:HG3	1:B:288:PHE:CZ	2.54	0.43
5:B:1353:TNL:H7C1	5:B:1353:TNL:O62	2.18	0.42
1:A:336:TYR:CZ	2:A:1351:FMN:HM72	2.54	0.42
1:B:336:TYR:CZ	2:B:1351:FMN:HM72	2.55	0.41
1:B:208:GLU:HG3	6:B:2216:HOH:O	2.19	0.41
1:B:248:ALA:HB2	1:B:274:ILE:HG23	2.03	0.41

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	351/362 (97%)	337 (96%)	13 (4%)	1 (0%)	41 24
1	B	351/362 (97%)	337 (96%)	13 (4%)	1 (0%)	41 24
All	All	702/724 (97%)	674 (96%)	26 (4%)	2 (0%)	41 24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	286	GLU
1	A	286	GLU

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	270/281 (96%)	269 (100%)	1 (0%)	91 87
1	B	272/281 (97%)	271 (100%)	1 (0%)	91 87
All	All	542/562 (96%)	540 (100%)	2 (0%)	91 87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	PHE

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Mol	Chain	Res	Type
1	B	311	PHE

Some 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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FMN	B	1351	-	31,33,33	1.37	3 (9%)	40,50,50	1.58	5 (12%)
2	FMN	A	1351	-	31,33,33	1.23	3 (9%)	40,50,50	1.48	6 (15%)
5	TNL	B	1353	-	11,16,16	2.30	3 (27%)	11,23,23	1.78	3 (27%)
3	GOL	A	1352	-	5,5,5	0.40	0	5,5,5	0.31	0
4	SO4	A	1353	-	4,4,4	0.16	0	6,6,6	0.17	0
4	SO4	A	1354	-	4,4,4	0.17	0	6,6,6	0.12	0
4	SO4	B	1352	-	4,4,4	0.15	0	6,6,6	0.10	0
5	TNL	A	1355	-	11,16,16	2.52	3 (27%)	11,23,23	1.86	3 (27%)

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	FMN	B	1351	-	-	1/18/18/18	0/3/3/3
2	FMN	A	1351	-	-	1/18/18/18	0/3/3/3
5	TNL	B	1353	-	-	6/6/12/12	0/1/1/1
5	TNL	A	1355	-	-	4/6/12/12	0/1/1/1
3	GOL	A	1352	-	-	0/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1355	TNL	O61-N6	4.70	1.30	1.22
5	A	1355	TNL	O41-N4	4.57	1.30	1.22
5	A	1355	TNL	O21-N2	4.52	1.30	1.22
2	B	1351	FMN	C10-N1	4.40	1.38	1.33
5	B	1353	TNL	O61-N6	4.35	1.30	1.22
5	B	1353	TNL	O21-N2	4.19	1.29	1.22
5	B	1353	TNL	O41-N4	3.37	1.28	1.22
2	A	1351	FMN	C10-N1	3.27	1.37	1.33
2	B	1351	FMN	C4A-N5	3.14	1.37	1.33
2	A	1351	FMN	C4-N3	3.08	1.38	1.33
2	A	1351	FMN	C4A-N5	2.87	1.37	1.33
2	B	1351	FMN	C4-N3	2.75	1.37	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1351	FMN	C4-N3-C2	6.27	120.44	115.14
5	B	1353	TNL	C6-C1-C2	4.47	119.72	113.26
2	A	1351	FMN	C4A-N5-C5A	4.08	120.85	116.77
2	A	1351	FMN	C4-N3-C2	4.08	118.58	115.14
2	B	1351	FMN	C4A-N5-C5A	4.06	120.83	116.77
5	A	1355	TNL	C6-C1-C2	3.86	118.83	113.26
2	A	1351	FMN	C10-C4A-N5	-3.52	118.83	121.26
2	B	1351	FMN	C1'-N10-C9A	3.22	120.83	118.29
2	B	1351	FMN	C4A-C4-N3	-3.20	119.05	123.43
2	A	1351	FMN	C4A-C4-N3	-2.54	119.96	123.43
5	A	1355	TNL	C3-C2-C1	-2.39	119.31	124.59
2	B	1351	FMN	C10-C4A-N5	-2.39	119.61	121.26
5	B	1353	TNL	C3-C2-C1	-2.28	119.56	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1353	TNL	C5-C6-C1	-2.21	119.72	124.59
2	A	1351	FMN	C1'-N10-C9A	2.16	119.99	118.29
5	A	1355	TNL	O41-N4-C4	2.13	121.81	118.80
2	A	1351	FMN	C1'-N10-C10	2.09	120.28	118.41

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1353	TNL	C1-C2-N2-O21
5	B	1353	TNL	C3-C2-N2-O21
5	A	1355	TNL	C3-C4-N4-O41
5	A	1355	TNL	C5-C4-N4-O41
5	B	1353	TNL	C5-C6-N6-O61
5	B	1353	TNL	C5-C4-N4-O41
5	B	1353	TNL	C3-C4-N4-O41
2	B	1351	FMN	C4'-C5'-O5'-P
2	A	1351	FMN	C4'-C5'-O5'-P
5	A	1355	TNL	C3-C2-N2-O21
5	B	1353	TNL	C1-C6-N6-O61
5	A	1355	TNL	C5-C6-N6-O61

There are no ring outliers.

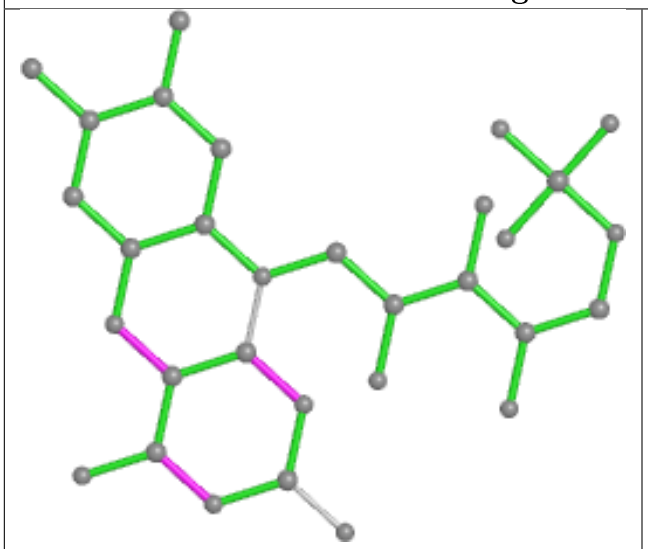
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1351	FMN	4	0
2	A	1351	FMN	4	0
5	B	1353	TNL	8	0
5	A	1355	TNL	8	0

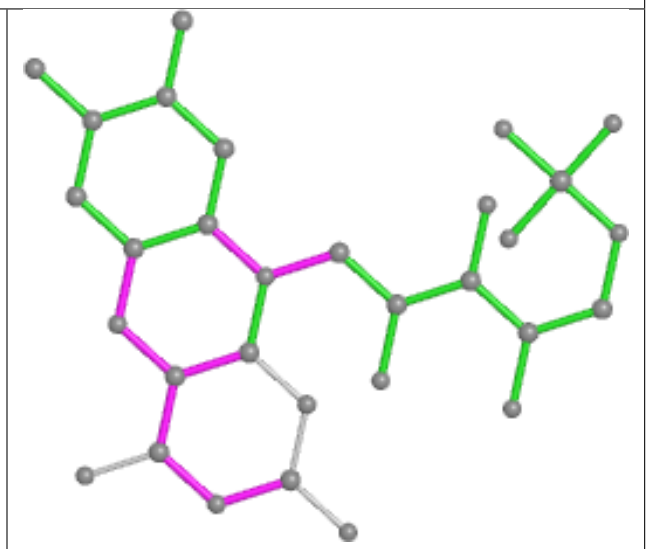
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

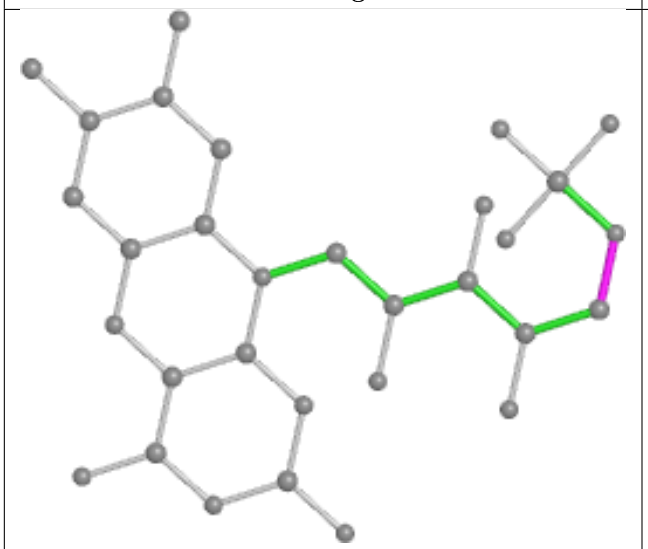
Ligand FMN B 1351



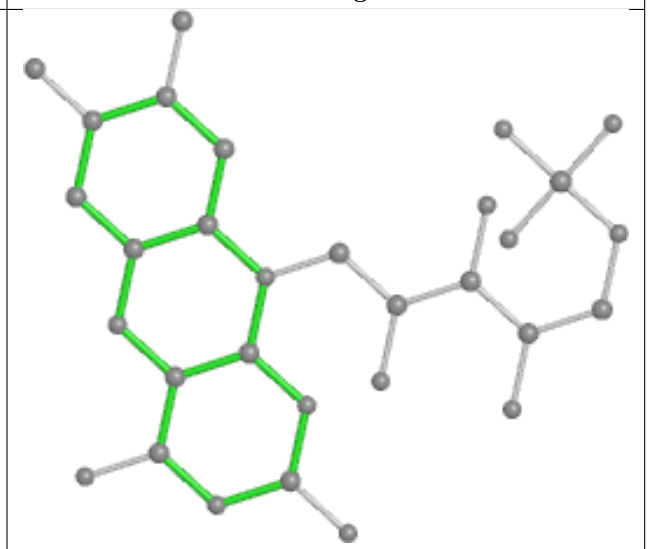
Bond lengths



Bond angles

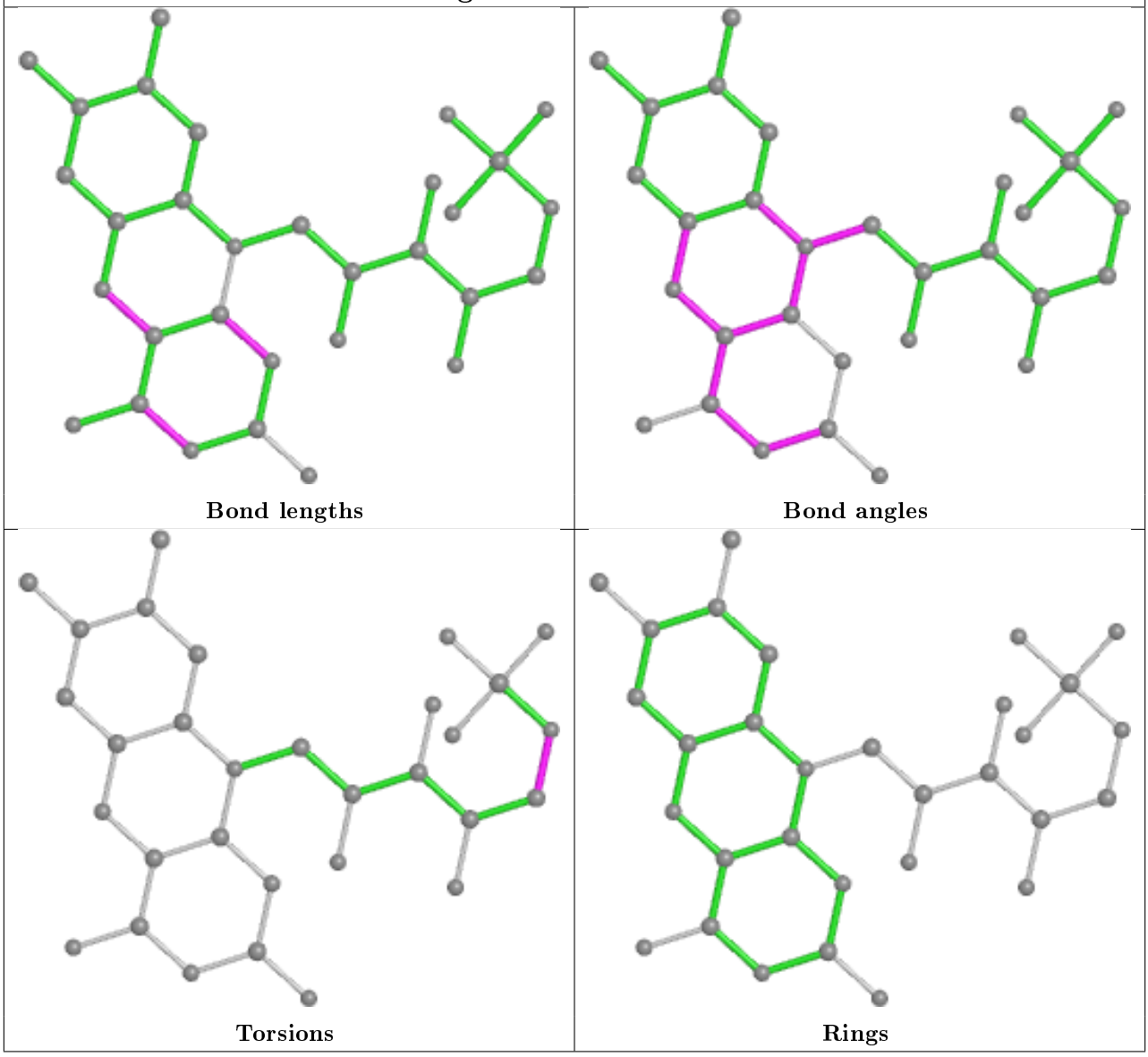


Torsions



Rings

Ligand FMN A 1351



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	349/362 (96%)	-0.02	6 (1%)	70	74	6, 10, 21, 45	0
1	B	349/362 (96%)	0.11	11 (3%)	47	52	6, 11, 25, 47	0
All	All	698/724 (96%)	0.04	17 (2%)	59	63	6, 11, 23, 47	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	LYS	4.0
1	B	132	ARG	3.4
1	B	192	THR	3.3
1	A	130	LEU	3.2
1	B	112	ASN	3.2
1	B	350	LYS	3.1
1	B	134	LEU	3.1
1	A	134	LEU	3.0
1	A	133	PRO	2.8
1	B	130	LEU	2.7
1	B	131	VAL	2.7
1	B	133	PRO	2.7
1	A	132	ARG	2.5
1	B	127	HIS	2.5
1	B	126	GLY	2.2
1	B	299	SER	2.1
1	A	127	HIS	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 carbohydrates in this entry.

6.4 Ligands (i)

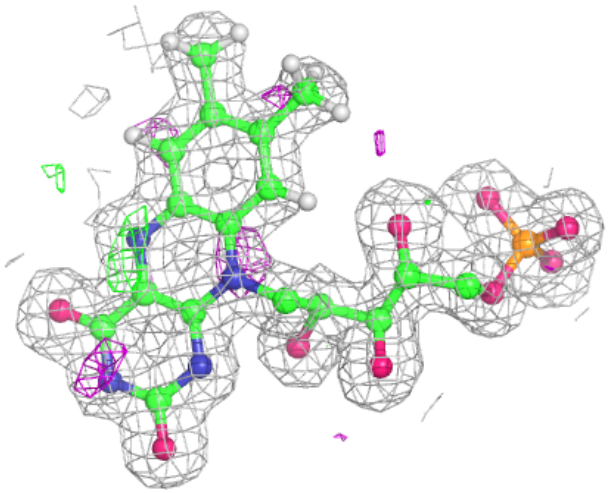
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

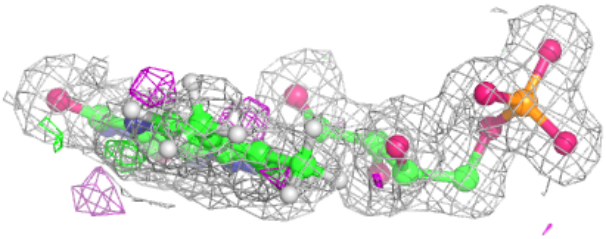
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	TNL	A	1355	16/16	0.76	0.43	14,41,50,55	0
5	TNL	B	1353	16/16	0.78	0.34	17,42,51,51	0
4	SO4	B	1352	5/5	0.92	0.30	43,45,46,46	0
3	GOL	A	1352	6/6	0.93	0.12	14,18,26,26	0
4	SO4	A	1353	5/5	0.95	0.11	33,37,39,41	0
4	SO4	A	1354	5/5	0.95	0.20	33,38,42,42	0
2	FMN	B	1351	31/31	0.95	0.09	4,8,12,16	0
2	FMN	A	1351	31/31	0.95	0.09	3,8,14,14	0

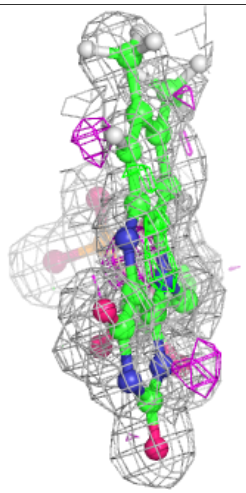
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN B 1351:

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

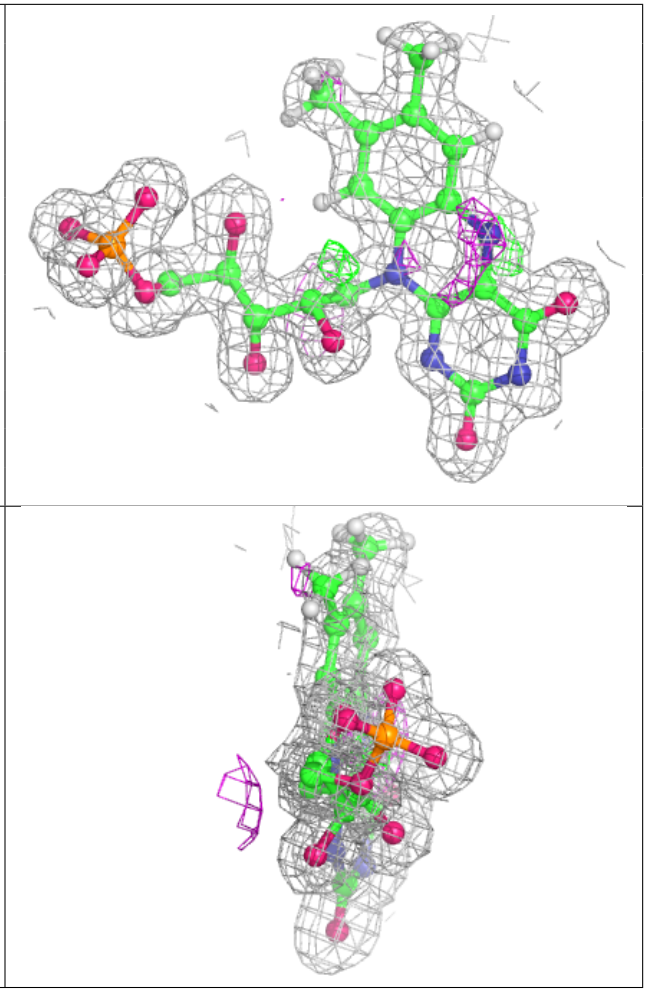






Electron density around FMN A 1351:

$2mF_o$-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.