

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 - 03:13 am BST

:	1AL8
:	THREE-DIMENSIONAL STRUCTURE OF GLYCOLATE OXIDASE WITH
	BOUND ACTIVE-SITE INHIBITORS
:	Stenberg, K.; Lindqvist, Y.
:	1997-06-12
:	2.20 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 (1)) were used in the production of this report:

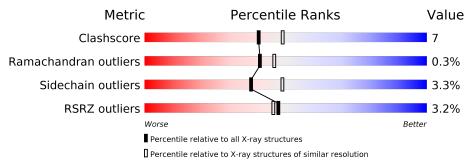
MolProbity		4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	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 2.20 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	$5594 \ (2.20-2.20)$
Ramachandran outliers	138981	5503(2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	А	359	3% 	16%	
T	Л	000	79%	16%	••

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
2	FMN	А	360	Х	-	-	-



2 Entry composition (i)

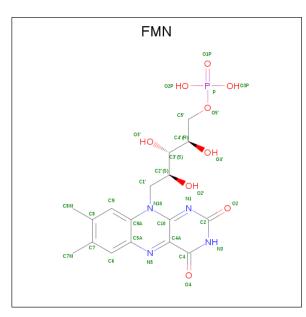
There are 4 unique types of molecules in this entry. The entry contains 2766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCOLATE OXIDASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	344	Total 2649	C 1692	N 459	O 485	S 13	0	0	0

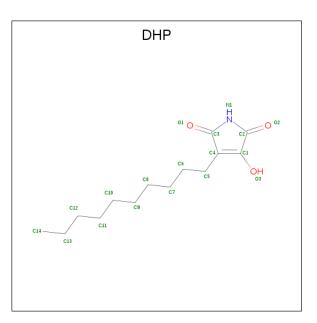
• Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	А	1	Total 31	С 17	N 4	0 9	Р 1	0	0

• Molecule 3 is 3-DECYL-2,5-DIOXO-4-HYDROXY-3-PYRROLINE (three-letter code: DHP) (formula: C₁₄H₂₃NO₃).





Mol	Chain	Residues					ZeroOcc	AltConf
2	Δ	1	Total	С	Ν	Ο	2	0
0	A		18	14	1	3	2	0

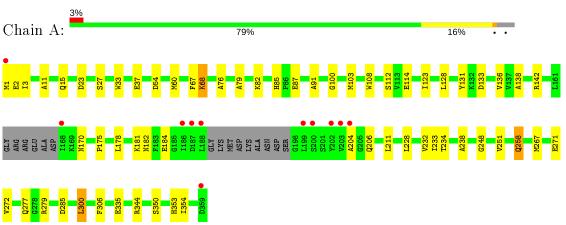
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	68	Total O 68 68	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: GLYCOLATE OXIDASE



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	I 4	Depositor	
Cell constants	95.40\AA 95.40\AA 93.50\AA	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	8.00 - 2.20	Depositor	
Resolution (A)	67.46 - 2.20	EDS	
% Data completeness	100.0 (8.00-2.20)	Depositor	
(in resolution range)	$98.6\ (67.46-2.20)$	EDS	
R _{merge}	(Not available)	Depositor	
R _{sym}	0.09	Depositor	
$\begin{array}{c c c c c c }\hline R_{sym} & \\ \hline & < I/\sigma(I) > {}^1 \end{array}$	$2.88 (at 2.20 \text{\AA})$	Xtriage	
Refinement program	X-PLOR 3.1	Depositor	
D D	0.194 , 0.251	Depositor	
R, R_{free}	0.180 , (Not available)	DCC	
R_{free} test set	No test flags present.	wwPDB-VP	
Wilson B-factor $(Å^2)$	25.2	Xtriage	
Anisotropy	0.131	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 49.0	EDS	
L-test for twinning ²	$< L > = 0.45, < L^2 > = 0.27$	Xtriage	
	0.026 for l,-k,h		
	0.036 for -l,-k,-h		
Estimated twinning fraction	0.029 for -h,-l,-k	Xtriage	
	0.026 for -h,l,k		
	0.098 for -k,-h,-l		
F_o, F_c correlation	0.95	EDS	
Total number of atoms	2766	wwPDB-VP	
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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, DHP

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).

Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.37	0/2696	0.65	0/3649	

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	А	2649	0	2710	38	0
2	А	31	0	18	1	0
3	А	18	0	22	0	0
4	А	68	0	0	2	0
All	All	2766	0	2750	39	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 7.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:A:67:PHE:HB3	1:A:123:ILE:HD13	1.66	0.77
1:A:300:LEU:HD13	1:A:354:ILE:HD11	1.68	0.74
1:A:54:ASP:O	1:A:344:ARG:HD3	1.90	0.71
1:A:33:TRP:CH2	1:A:37:GLU:HG3	2.30	0.66
1:A:23:ASP:O	1:A:27:SER:HB2	2.01	0.61
1:A:138:ALA:O	1:A:142:ARG:HG2	2.01	0.60
1:A:68:LYS:HB2	1:A:68:LYS:HZ3	1.69	0.56
1:A:108:TRP:CZ3	1:A:131:TYR:OH	2.61	0.54
1:A:175:PRO:HD2	1:A:178:LEU:HD12	1.92	0.52
1:A:100:GLY:HA2	4:A:416:HOH:O	2.12	0.50
1:A:238:ALA:HB2	1:A:272:VAL:HG13	1.94	0.50
1:A:1:MET:HG3	1:A:2:GLU:H	1.77	0.49
1:A:181:LYS:HA	1:A:184:GLU:HG2	1.95	0.49
1:A:3:ILE:HD12	1:A:3:ILE:N	2.27	0.49
1:A:108:TRP:HZ3	1:A:131:TYR:OH	1.93	0.49
1:A:60:MET:CE	1:A:335:GLU:HB2	2.42	0.49
1:A:76:ALA:HB2	1:A:306:PHE:HB3	1.94	0.48
1:A:85:HIS:HD2	1:A:87:GLU:H	1.60	0.48
1:A:79:ALA:CB	1:A:108:TRP:HB2	2.44	0.47
1:A:1:MET:HG3	1:A:2:GLU:N	2.30	0.47
1:A:68:LYS:HB2	1:A:68:LYS:NZ	2.30	0.47
2:A:360:FMN:H9	2:A:360:FMN:H1'2	1.66	0.46
1:A:79:ALA:HB1	1:A:108:TRP:HB2	1.97	0.46
1:A:267:MET:HG3	4:A:465:HOH:O	2.14	0.46
1:A:82:LYS:HA	1:A:85:HIS:O	2.15	0.46
1:A:133:ASP:OD2	1:A:136:VAL:HG23	2.17	0.45
1:A:181:LYS:HA	1:A:184:GLU:CG	2.47	0.45
1:A:285:ASP:HB3	1:A:306:PHE:HB2	2.00	0.44
1:A:277:GLN:HB3	1:A:279:ARG:HH11	1.84	0.43
1:A:112:SER:HA	1:A:182:ASN:OD1	2.19	0.42
1:A:232:VAL:O	1:A:251:VAL:HA	2.19	0.42
1:A:206:GLN:HA	1:A:206:GLN:NE2	2.35	0.42
1:A:233:ILE:HD12	1:A:234:THR:HG23	2.00	0.42
1:A:87:GLU:HB3	1:A:91:ALA:HB2	2.02	0.41
1:A:228:LEU:HD22	1:A:248:GLY:HA3	2.01	0.41
1:A:131:TYR:HA	1:A:206:GLN:O	2.21	0.41
1:A:350:SER:O	1:A:353:HIS:HB2	2.21	0.41
1:A:11:ALA:O	1:A:15:GLN:HG3	2.21	0.40
1:A:258:GLN:HB3	1:A:258:GLN:HE21	1.65	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	Analysed Favoured Allowed		Outliers	Percentiles	
1	А	338/359~(94%)	322~(95%)	15~(4%)	1 (0%)	41	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	204	ALA

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	Analysed Rotameric		Percentiles	
1	А	276/287~(96%)	267~(97%)	9~(3%)	38 49	

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

Mol	Chain	Res	Type
1	А	68	LYS
1	А	103	MET
1	А	114	GLU
1	А	128	LEU
1	А	170	ASN
1	А	211	LEU
1	А	258	GLN
1	А	271	GLU
1	А	300	LEU



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	7	ASN
1	А	57	ASN
1	А	85	HIS
1	А	258	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)

2 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	Turne	e Chain	Res	Link	Bond lengths			Bond angles		
	l Type Chain Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
3	DHP	А	361	-	18, 18, 18	4.11	6 (33%)	$18,\!22,\!22$	<mark>5.35</mark>	5 (27%)
2	FMN	А	360	-	31,33,33	2.90	8 (25%)	$40,\!50,\!50$	<mark>3.31</mark>	16 (40%)

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.



Ν	Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
	3	DHP	А	361	-	-	5/10/26/26	0/1/1/1
	2	FMN	А	360	-	2/2/4/4	9/18/18/18	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	Ideal(Å)
2	А	360	FMN	C1'-N10	-12.77	1.35	1.48
3	А	361	DHP	O1-C3	12.34	1.47	1.23
3	А	361	DHP	C3-C4	-6.79	1.35	1.48
3	А	361	DHP	O2-C2	6.61	1.36	1.23
2	А	360	FMN	C4-N3	5.14	1.42	1.33
3	А	361	DHP	C1-C2	-5.06	1.32	1.49
3	А	361	DHP	O3-C1	-4.50	1.18	1.33
2	А	360	FMN	C10-N1	3.89	1.38	1.33
2	А	360	FMN	O2'-C2'	-3.60	1.35	1.43
3	А	361	DHP	C2-N1	-2.67	1.32	1.38
2	А	360	FMN	C4A-N5	2.62	1.37	1.33
2	А	360	FMN	C2'-C3'	-2.45	1.48	1.53
2	А	360	FMN	C6-C5A	-2.37	1.38	1.41
2	А	360	FMN	C9A-C5A	-2.06	1.38	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	361	DHP	O1-C3-C4	19.20	148.88	128.04
2	А	360	FMN	C4-N3-C2	11.85	125.14	115.14
3	А	361	DHP	O1-C3-N1	-10.38	100.95	125.08
2	А	360	FMN	C4A-C4-N3	-7.40	113.31	123.43
2	А	360	FMN	O4'-C4'-C3'	5.94	123.53	109.10
2	А	360	FMN	C4-C4A-C10	5.87	123.84	119.95
2	А	360	FMN	C4'-C3'-C2'	4.42	122.56	113.36
2	А	360	FMN	C5A-C9A-N10	4.21	120.77	117.72
3	А	361	DHP	C4-C3-N1	4.19	110.16	106.78
2	А	360	FMN	P-O5'-C5'	4.15	129.72	118.30
2	А	360	FMN	O5'-C5'-C4'	3.86	119.66	109.36
2	А	360	FMN	C1'-N10-C9A	3.59	121.12	118.29
2	А	360	FMN	C1'-C2'-C3'	3.57	119.76	109.79
2	А	360	FMN	C4-C4A-N5	-3.41	114.70	118.60
3	А	361	DHP	C3-N1-C2	-3.40	107.69	111.29
2	А	360	FMN	C9A-N10-C10	-3.20	117.71	121.91
2	А	360	FMN	O2'-C2'-C1'	3.15	117.17	109.59
2	А	360	FMN	C1'-N10-C10	3.08	121.17	118.41
2	А	360	FMN	O3'-C3'-C4'	2.40	114.61	108.81
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	361	DHP	O3-C1-C2	2.40	128.02	120.16
2	А	360	FMN	O2P-P-O5'	-2.11	101.11	106.73

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom	
2	А	360	FMN	C4'	
2	А	360	FMN	C2'	

All (14) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	А	360	FMN	C2'-C1'-N10-C9A
2	А	360	FMN	N10-C1'-C2'-O2'
2	А	360	FMN	O3'-C3'-C4'-O4'
2	А	360	FMN	O4'-C4'-C5'-O5'
2	А	360	FMN	C4'-C5'-O5'-P
2	А	360	FMN	O2'-C2'-C3'-O3'
2	А	360	FMN	C2'-C3'-C4'-O4'
3	А	361	DHP	С11-С10-С9-С8
3	А	361	DHP	C10-C11-C12-C13
3	А	361	DHP	С6-С7-С8-С9
3	А	361	DHP	C9-C10-C11-C12
3	А	361	DHP	C11-C12-C13-C14
2	А	360	FMN	O3'-C3'-C4'-C5'
2	А	360	FMN	C3'-C4'-C5'-O5'

There are no ring outliers.

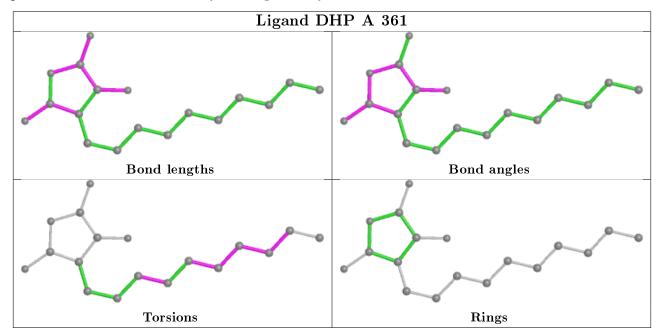
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	360	FMN	1	0

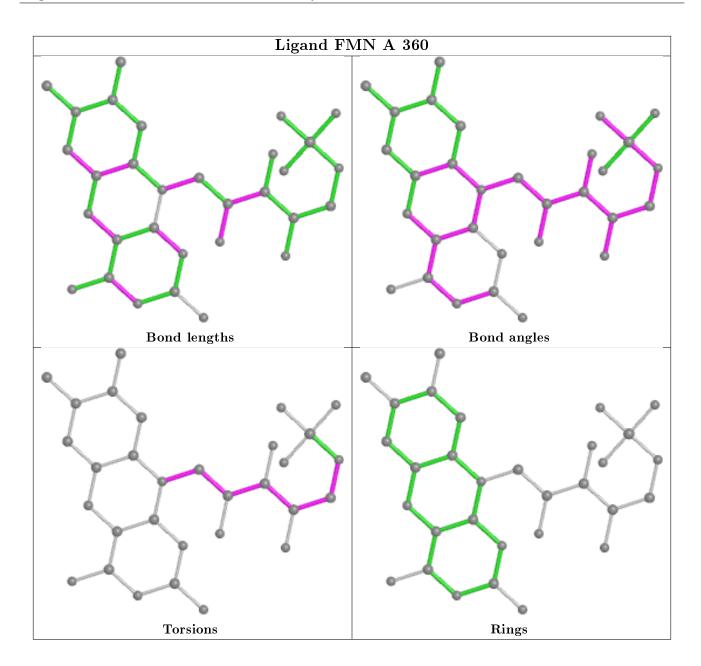
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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







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, 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		$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9	
1	А	344/359~(95%)	-0.56	11 (3%)	47	45	8, 22, 64, 131	0

All (11) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	А	202	TYR	7.3
1	А	1	MET	5.2
1	А	200	SER	5.0
1	А	199	LEU	4.4
1	А	188	LEU	3.6
1	А	203	VAL	3.0
1	А	186	ILE	2.7
1	А	187	ASP	2.6
1	А	168	ILE	2.6
1	А	204	ALA	2.6
1	А	359	ASP	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)

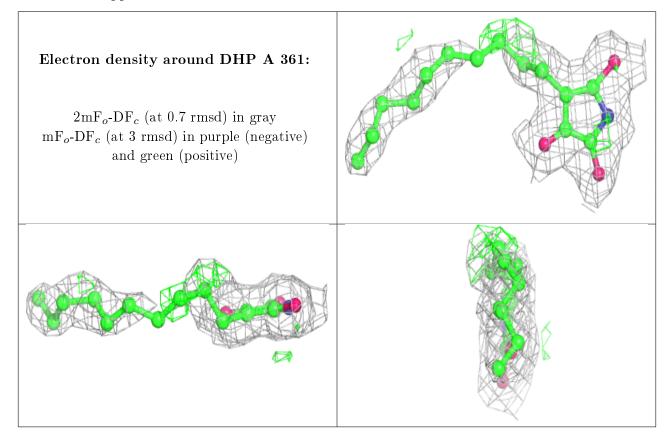
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



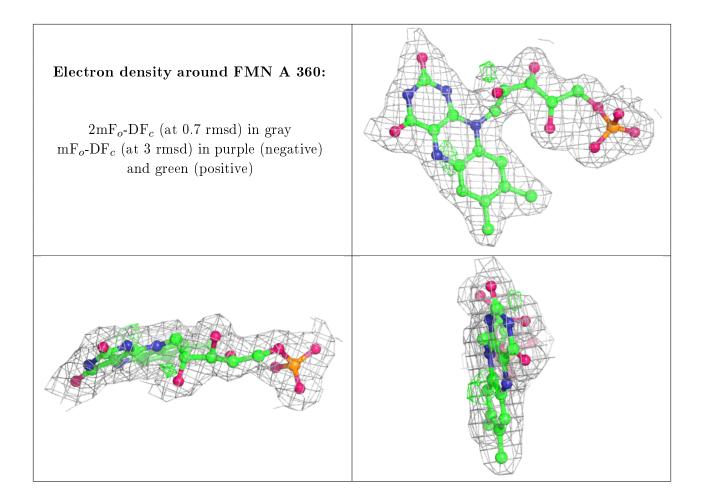
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DHP	А	361	18/18	0.96	0.13	$13,\!23,\!34,\!34$	2
2	FMN	А	360	31/31	0.98	0.08	$9,\!15,\!18,\!18$	0

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.

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







6.5 Other polymers (i)

There are no such residues in this entry.

