

Full wwPDB X-ray Structure Validation Report (i)

May 19, 2020 – 07:42 pm BST

PDB ID : 2Z6I

Title : Crystal Structure of S. pneumoniae Enoyl-Acyl Carrier Protein Reductase

(FabK)

Authors: Saito, J.; Yamada, M.; Watanabe, T.; Takeuchi, Y.

Deposited on : 2007-08-01

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 (1)) 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)

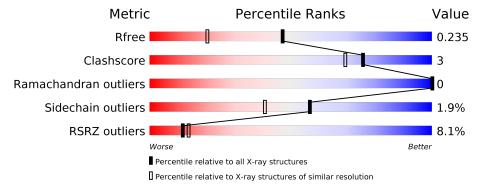
Validation Pipeline (wwPDB-VP) : 2.11

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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
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	332	89%	5% • 5%
1	В	332	7% 89%	7% • •



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5170 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 Trans-2-enoyl-ACP reductase II.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	317	Total	С	N	О	Se	0	0	0
1	Λ	911	2342	1487	399	446	10	0	U	
1	D	321	Total	С	N	О	Se	0	0	0
1	D	321	2373	1506	403	454	10	0	0	U

There are 16 discrepancies between the modelled and reference sequences:

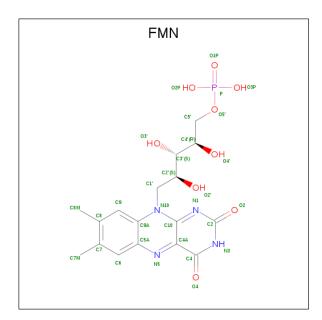
Chain	Residue	Modelled	Actual	Comment	Reference
A	325	LEU	=	EXPRESSION TAG	UNP Q9FBC5
A	326	GLU	-	EXPRESSION TAG	UNP Q9FBC5
A	327	HIS	_	EXPRESSION TAG	UNP Q9FBC5
A	328	HIS	_	EXPRESSION TAG	UNP Q9FBC5
A	329	HIS	_	EXPRESSION TAG	UNP Q9FBC5
A	330	HIS	_	EXPRESSION TAG	UNP Q9FBC5
A	331	HIS	-	EXPRESSION TAG	UNP Q9FBC5
A	332	HIS	_	EXPRESSION TAG	UNP Q9FBC5
В	325	LEU	-	EXPRESSION TAG	UNP Q9FBC5
В	326	GLU	-	EXPRESSION TAG	UNP Q9FBC5
В	327	HIS	_	EXPRESSION TAG	UNP Q9FBC5
В	328	HIS	-	EXPRESSION TAG	UNP Q9FBC5
В	329	HIS	_	EXPRESSION TAG	UNP Q9FBC5
В	330	HIS	=	EXPRESSION TAG	UNP Q9FBC5
В	331	HIS	-	EXPRESSION TAG	UNP Q9FBC5
В	332	HIS	-	EXPRESSION TAG	UNP Q9FBC5

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	3	Total Ca 3 3	0	0
2	A	3	Total Ca 3 3	0	0

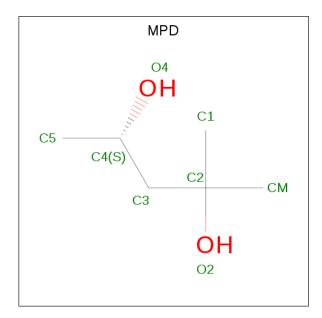


 $\bullet \ \ Molecule\ 3\ is\ FLAVIN\ MONONUCLEOTIDE\ (three-letter\ code:\ FMN)\ (formula:\ C_{17}H_{21}N_4O_9P).$



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	Λ	1	Total	С	N	О	Р	0	0
)	3 A	1	31	17	4	9	1	U	
9	D	1	Total	С	N	О	Р	0	0
3	Б	1	31	17	4	9	1	U	U

• Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).





Mol	Chain	Residues	${f Atoms}$		ZeroOcc	AltConf
4	A	1	Total C O 8 6 2		0	0

$\bullet\,$ Molecule 5 is water.

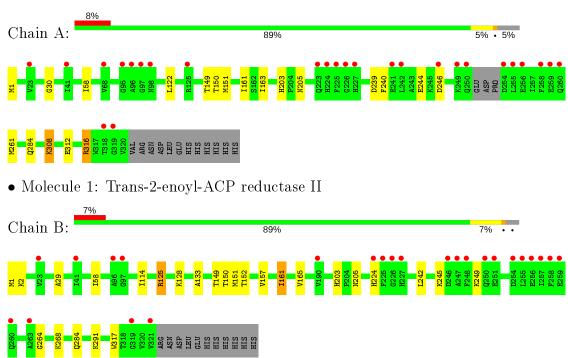
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	188	Total O 188 188	0	0
5	В	191	Total O 191 191	0	0



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: Trans-2-enoyl-ACP reductase II





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	50.39Å 126.89Å 53.34Å	Depositor
a, b, c, α , β , γ	90.00° 111.54° 90.00°	Depositor
Resolution (Å)	29.14 - 1.70	Depositor
Resolution (A)	28.40 - 1.70	EDS
% Data completeness	99.7 (29.14-1.70)	Depositor
(in resolution range)	99.7 (28.40-1.70)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.09 \; ({\rm at} \; 1.70 {\rm \AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.202 , 0.235	Depositor
it, it free	0.203 , 0.235	DCC
R_{free} test set	3379 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.40 , 50.1	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5170	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 5.74% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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, CA, MPD

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		
Moi Chain		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.46	0/2365	0.55	0/3174	
1	В	0.44	0/2398	0.56	0/3222	
All	All	0.45	0/4763	0.55	0/6396	

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	2342	0	2403	17	0
1	В	2373	0	2430	21	0
2	A	3	0	0	0	0
2	В	3	0	0	0	0
3	A	31	0	19	0	0
3	В	31	0	19	0	0
4	A	8	0	14	0	0
5	A	188	0	0	1	0
5	В	191	0	0	1	0
All	All	5170	0	4885	30	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 (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		${\rm distance}\;({\rm \AA})$	overlap (Å)
1:A:203:HIS:HD2	1:A:205:ASN:H	1.18	0.87
1:B:203:HIS:HD2	1:B:205:ASN:H	1.21	0.83
1:A:316:ARG:O	1:B:1:MSE:HG3	1.87	0.73
1:B:161:ILE:HD11	1:B:165:VAL:CG2	2.22	0.70
1:B:203:HIS:CD2	1:B:205:ASN:H	2.10	0.66
1:A:149:THR:H	1:B:284:GLN:HE22	1.50	0.60
1:A:203:HIS:CD2	1:A:205:ASN:H	2.11	0.58
1:A:151:MSE:HG3	1:B:150:THR:HB	1.85	0.58
1:A:284:GLN:HE22	1:B:149:THR:H	1.51	0.57
1:A:239:ASP:HB3	1:A:261:MSE:CE	2.36	0.56
1:A:239:ASP:HB3	1:A:261:MSE:HE2	1.88	0.55
1:A:150:THR:HB	1:B:151:MSE:HG3	1.88	0.55
1:A:151:MSE:HG2	1:B:151:MSE:HG2	1.92	0.52
1:A:308:LYS:O	1:A:312:GLU:HG3	2.10	0.52
1:A:30:GLY:HA2	1:A:58:ILE:HG13	1.91	0.51
1:B:125:ARG:HG2	5:B:530:HOH:O	2.10	0.51
5:A:751:HOH:O	1:B:224:HIS:HD2	1.93	0.50
1:B:264:GLY:O	1:B:268:LYS:HG3	2.13	0.49
1:A:161:ILE:HD12	1:A:163:ILE:CG1	2.43	0.49
1:B:157:VAL:O	1:B:161:ILE:HD13	2.11	0.49
1:B:114:ILE:HG12	1:B:133:ALA:HB3	1.96	0.47
1:B:1:MSE:HG2	1:B:2:LYS:N	2.29	0.47
1:A:30:GLY:CA	1:A:58:ILE:HG13	2.47	0.45
1:B:161:ILE:HD11	1:B:165:VAL:HG22	1.97	0.45
1:B:157:VAL:O	1:B:161:ILE:CD1	2.66	0.43
1:A:1:MSE:HE3	1:B:317:TRP:CZ2	2.53	0.42
1:B:245:LYS:O	1:B:249:LYS:HG2	2.18	0.42
1:A:284:GLN:HB2	1:B:152:THR:HG21	2.01	0.42
1:B:29:ALA:HB3	1:B:58:ILE:HD11	2.01	0.41
1:A:240:PHE:O	1:A:244:GLU:HG3	2.22	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	Perce	$_{ m ntiles}$
1	A	313/332 (94%)	307 (98%)	6 (2%)	0	100	100
1	В	319/332 (96%)	313 (98%)	6 (2%)	0	100	100
All	All	$632/664 \ (95\%)$	620 (98%)	12 (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	$237/242 \ (98\%)$	233 (98%)	4 (2%)	60 46
1	В	241/242 (100%)	236 (98%)	5 (2%)	53 36
All	All	478/484 (99%)	469 (98%)	9 (2%)	57 41

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

Mol	Chain	Res	Type
1	A	122	LEU
1	A	246	ASP
1	A	308	LYS
1	A	316	ARG
1	В	125	ARG
1	В	128	LYS
1	В	161	ILE
1	В	242	LEU

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	В	291	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	HIS
1	A	224	HIS
1	A	260	GLN
1	A	284	GLN
1	A	311	GLN
1	В	144	HIS
1	В	203	HIS
1	В	224	HIS
1	В	284	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)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	Tuno	Chain	Dog Limb		Res	Link	Bo	nd leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
4	MPD	A	601	-	7,7,7	0.25	0	9,10,10	0.39	0		
3	FMN	A	401	-	31,33,33	1.56	5 (16%)	40,50,50	1.83	7 (17%)		
3	FMN	В	402	-	31,33,33	1.51	5 (16%)	40,50,50	1.76	8 (20%)		

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	${f Torsions}$	Rings
4	MPD	A	601	_	-	1/5/5/5	-
3	FMN	A	401	_	-	1/18/18/18	0/3/3/3
3	FMN	В	402	_	_	1/18/18/18	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
3	A	401	FMN	C10-N1	4.53	1.39	1.33
3	В	402	FMN	C10-N1	4.24	1.38	1.33
3	В	402	FMN	C4-N3	3.79	1.39	1.33
3	A	401	FMN	C4A-N5	3.67	1.38	1.33
3	A	401	FMN	C4-N3	3.54	1.39	1.33
3	В	402	FMN	C4A-N5	3.19	1.37	1.33
3	В	402	FMN	C1'-N10	2.99	1.51	1.48
3	A	401	FMN	C1'-N10	2.94	1.51	1.48
3	В	402	FMN	C5A-N5	2.23	1.39	1.35
3	A	401	FMN	C5A-N5	2.10	1.38	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
3	В	402	FMN	C4-N3-C2	6.41	120.55	115.14
3	A	401	FMN	C4-N3-C2	6.30	120.46	115.14
3	A	401	FMN	C4A-N5-C5A	4.19	120.95	116.77
3	A	401	FMN	C1'-N10-C9A	4.02	121.45	118.29
3	A	401	FMN	C10-C4A-N5	-3.44	118.88	121.26
3	В	402	FMN	C4A-N5-C5A	3.43	120.20	116.77
3	В	402	FMN	C5A-C9A-N10	3.37	120.16	117.72
3	В	402	FMN	C4A-C4-N3	-3.05	119.27	123.43
3	A	401	FMN	C4A-C4-N3	-2.94	119.41	123.43
3	В	402	FMN	C10-C4A-N5	-2.89	119.26	121.26
3	A	401	FMN	C5A-C9A-N10	2.70	119.67	117.72

Continued on next page...



$\alpha \cdots \tau$	e	•	
Continued	trom	mraniaone	maaa
-	110116	predidus	puyc

Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^{o})$
3	В	402	FMN	C1'-N10-C9A	2.35	120.15	118.29
3	В	402	FMN	C9A-N10-C10	-2.11	119.14	121.91
3	В	402	FMN	O3'-C3'-C2'	2.10	113.89	108.81
3	A	401	FMN	C4-C4A-N5	2.10	120.99	118.60

There are no chirality outliers.

All (3) torsion outliers are listed below:

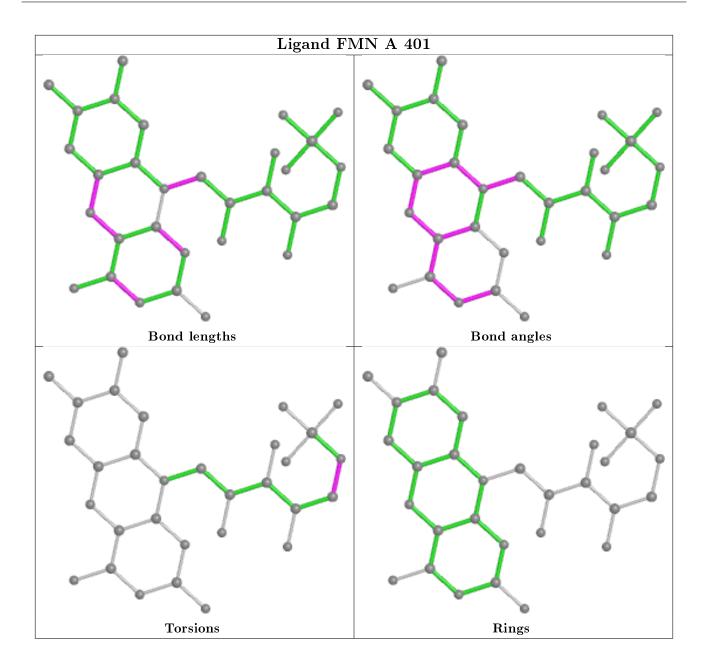
Mol	Chain	Res	Type	Atoms
3	A	401	FMN	C4'-C5'-O5'-P
4	A	601	MPD	O2-C2-C3-C4
3	В	402	FMN	C4'-C5'-O5'-P

There are no ring outliers.

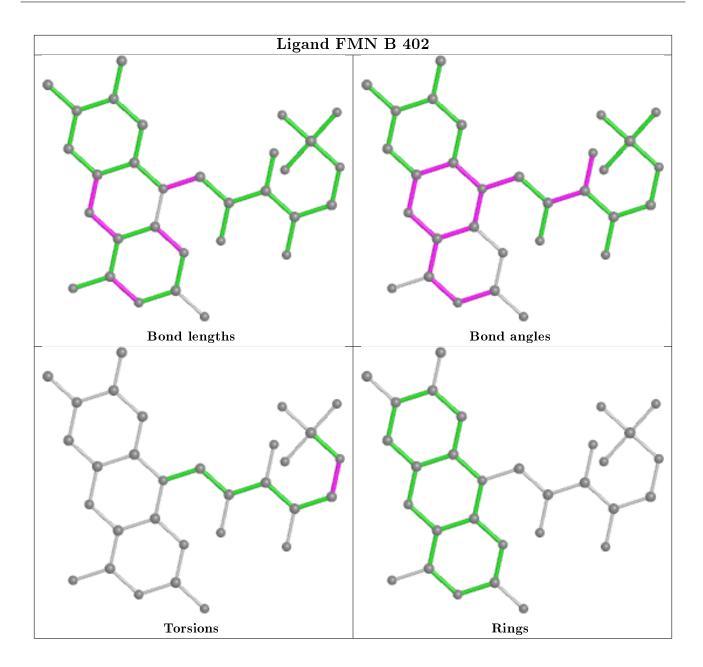
No monomer is involved in short contacts.

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 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	${f Analysed}$	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	$307/332 \ (92\%)$	0.43	26 (8%) 10 12	9, 16, 32, 48	0
1	В	311/332 (93%)	0.38	24 (7%) 13 15	9, 16, 31, 43	0
All	All	618/664 (93%)	0.40	50 (8%) 12 14	9, 16, 31, 48	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	96	ALA	7.5
1	A	255	LEU	6.7
1	A	225	PHE	6.4
1	A	96	ALA	5.9
1	A	319	GLY	5.2
1	В	255	LEU	5.2
1	В	225	PHE	4.8
1	A	97	GLY	4.7
1	В	227	HIS	4.6
1	A	250	GLN	4.6
1	A	224	HIS	4.4
1	В	263	ALA	4.1
1	В	257	ILE	4.0
1	В	321	VAL	3.8
1	В	259	GLU	3.7
1	A	260	GLN	3.6
1	В	256	GLU	3.6
1	A	226	GLY	3.5
1	A	254	ASP	3.5
1	В	248	PHE	3.5
1	В	247	ALA	3.5
1	A	227	HIS	3.4
1	В	97	GLY	3.3
1	В	41	ILE	3.2

Continued on next page...



Continued from previous page...

Mol	Mol Chain		Type	RSRZ	
1	A	259	GLU	3.2	
1	A	256	GLU	3.1	
1	A	242	LEU	3.1	
1	В	251	GLU	3.0	
1	В	226	GLY	3.0	
1	A	125	ARG	2.9	
1	В	254	ASP	2.9	
1	В	319	GLY	2.8	
1	В	260	GLN	2.8	
1	A	246	ASP	2.8	
1	A	318	THR	2.7	
1	A	68	VAL	2.6	
1	В	258	PHE	2.6	
1	A	258	PHE	2.5	
1	В	190	VAL	2.5	
1	A	98	ASN	2.5	
1	A	223	GLN	2.5	
1	A	41	ILE	2.5	
1	A	241	GLU	2.2	
1	В	250	GLN	2.2	
1	В	246	ASP	2.2	
1	В	23	VAL	2.2	
1	A	249	LYS	2.1	
1	A	23	VAL	2.0	
1	В	224	HIS	2.0	
1	A	95	GLY	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.

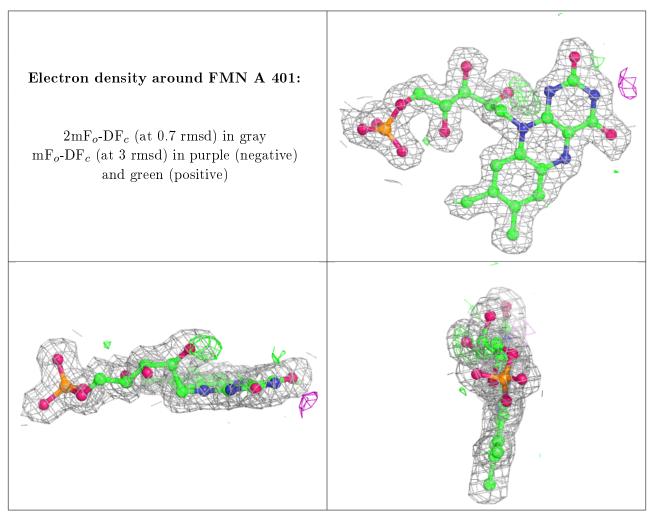
6.4 Ligands (i)

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, 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.

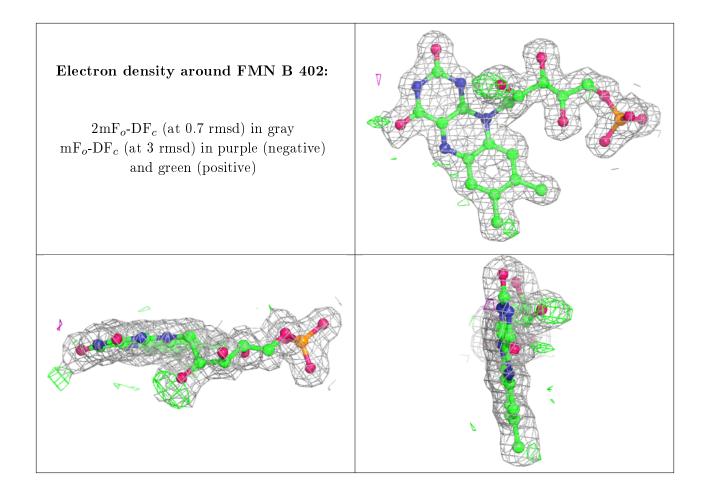


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	MPD	A	601	8/8	0.88	0.12	30,30,31,31	0
3	FMN	A	401	31/31	0.95	0.11	8,11,13,14	0
3	FMN	В	402	31/31	0.96	0.10	8,13,14,15	0
2	CA	В	505	1/1	0.97	0.05	14,14,14,14	1
2	CA	A	506	1/1	0.99	0.04	12,12,12,12	1
2	CA	В	501	1/1	0.99	0.04	14,14,14,14	0
2	CA	В	504	1/1	0.99	0.03	15,15,15,15	0
2	CA	A	503	1/1	0.99	0.03	15,15,15,15	0
2	CA	A	502	1/1	0.99	0.04	17,17,17,17	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 (i)

There are no such residues in this entry.

