

Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2020 - 09:20 AM BST

PDB ID : 6GAR

Title : Crystal structure of oxidised ferredoxin/flavodoxin NADP+ oxidoreductase 1

(FNR1) from Bacillus cereus

Authors: Skramo, S.; Gudim, I.; Hersleth, H.-P.

Deposited on : 2018-04-12

Resolution : 2.40 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:

Mol Probity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as 541 be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.13.1 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)

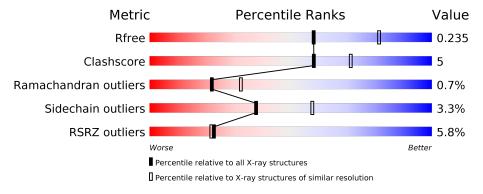
Validation Pipeline (wwPDB-VP) : 2.13.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	349	5% 88%	10%			
1	В	349	7% 80%	17%			



2 Entry composition (i)

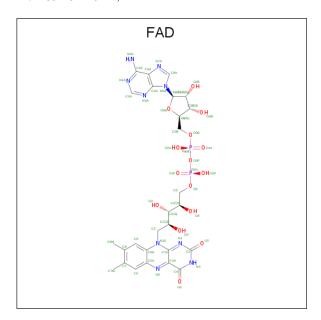
There are 6 unique types of molecules in this entry. The entry contains 5677 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ferredoxin–NADP reductase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	346	Total 2698	C 1710	N 455	O 526	S 7	0	0	0
1	В	343	Total 2671	C 1694	N 451	O 520	S 6	0	0	0

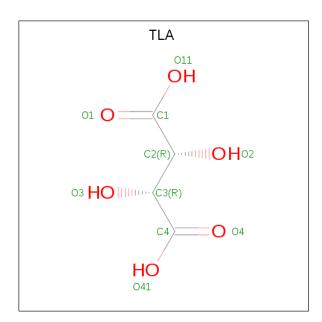
• Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	Λ.	1	Total C N O P		0	0			
	2 A	1	53	27	9	15	2	U	
2	D	1	Total	С	N	О	Р	0	0
2	Б	1	53	27	9	15	2	U	0

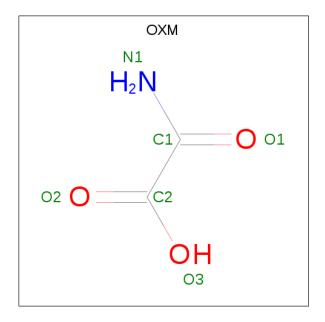
• Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 4 6	0	0

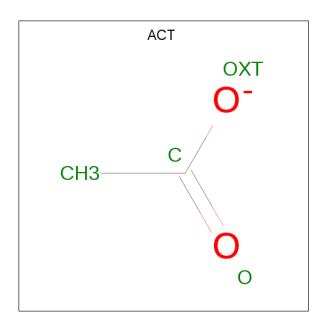
• Molecule 4 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1		2	1	3	0	0
4	В	1	Total 6	C 2	N 1	O 3	0	0

 \bullet Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $\mathrm{C_2H_3O_2}).$





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	В	1	Total C 4 2	O 2	0	0

• Molecule 6 is water.

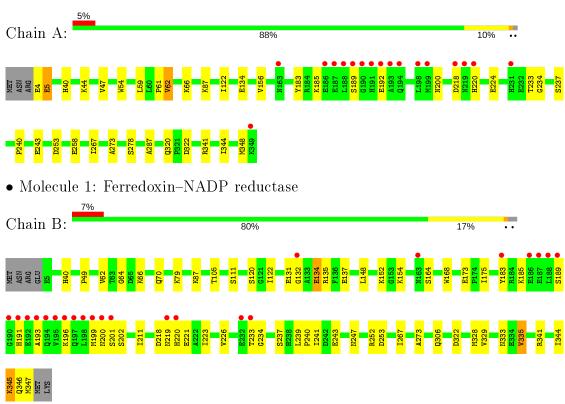
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
6	A	88	Total O 88 88	0	0
6	В	88	Total O 88 88	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Ferredoxin–NADP reductase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	57.17Å 164.33Å 95.01Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 - 2.40	Depositor
Resolution (A)	48.98 - 2.40	EDS
% Data completeness	98.3 (48.98-2.40)	Depositor
(in resolution range)	98.4 (48.98-2.40)	EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.13 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
D D.	0.186 , 0.235	Depositor
R, R_{free}	0.186 , 0.235	DCC
R_{free} test set	1709 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 46.4	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5677	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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 40.96 % 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 2.5342e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: OXM, TLA, FAD, ACT

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	0.42	0/2747	0.57	0/3707	
1	В	0.43	0/2720	0.59	0/3674	
All	All	0.43	0/5467	0.58	0/7381	

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2698	0	2684	18	0
1	В	2671	0	2656	32	0
2	A	53	0	31	1	0
2	В	53	0	31	1	0
3	A	10	0	4	1	0
4	A	6	0	2	0	0
4	В	6	0	2	0	0
5	В	4	0	3	0	0
6	A	88	0	0	1	0
6	В	88	0	0	3	0
All	All	5677	0	5413	52	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 5.

All (52) 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:B:66:LYS:HE3	1:B:70:GLN:HE21	1.35	0.89
1:A:348:MET:HE3	1:B:152:LYS:HB2	1.68	0.76
1:B:344:ILE:O	1:B:346:GLN:N	2.24	0.69
1:A:62:VAL:HG13	1:A:66:LYS:HB3	1.75	0.68
1:B:135:ARG:HH21	1:B:221:GLU:HG3	1.64	0.63
1:B:62:VAL:HG13	1:B:66:LYS:HB3	1.81	0.62
1:A:4:GLU:HG2	1:A:5:GLU:H	1.64	0.62
1:B:239:LEU:HD12	1:B:240:PRO:HD2	1.82	0.60
1:B:148:LEU:HB3	1:B:175:ILE:HD13	1.85	0.59
1:A:134:GLU:CD	1:A:134:GLU:H	2.06	0.59
1:B:120:SER:O	1:B:252:ARG:NH1	2.36	0.58
1:A:267:ILE:HG13	1:A:273:ALA:HB2	1.85	0.58
2:A:401:FAD:O2'	2:A:401:FAD:H5'2	2.03	0.57
1:B:211:ILE:HG23	1:B:226:VAL:HG13	1.87	0.56
1:B:40:HIS:HB3	6:B:587:HOH:O	2.06	0.54
1:B:168:TRP:CZ3	1:B:247:ASN:HB2	2.43	0.54
1:B:341:ARG:CZ	1:B:345:LYS:HE2	2.40	0.52
1:B:223:ILE:HG22	1:B:241:ILE:HD11	1.93	0.51
1:A:122:ILE:HB	1:A:253:ASP:HB3	1.92	0.51
1:A:233:THR:OG1	1:A:234:GLY:N	2.42	0.51
1:A:156:VAL:HG12	1:A:243:GLU:HB2	1.91	0.51
2:B:401:FAD:O2'	2:B:401:FAD:H5'2	2.10	0.51
1:B:322:ASP:OD1	1:B:322:ASP:N	2.40	0.49
1:B:233:THR:OG1	1:B:234:GLY:N	2.46	0.49
1:A:54:TRP:CZ3	1:A:61:PRO:HG3	2.47	0.49
1:B:173:GLU:HB3	6:B:562:HOH:O	2.11	0.49
1:A:344:ILE:O	1:A:348:MET:HG2	2.12	0.49
1:A:40:HIS:HB3	6:A:565:HOH:O	2.14	0.48
1:B:267:ILE:HG13	1:B:273:ALA:HB2	1.98	0.46
1:A:220:HIS:NE2	1:A:224:GLU:OE2	2.48	0.46
1:B:183:TYR:CE2	1:B:185:LYS:HB2	2.51	0.46
1:B:134:GLU:HA	1:B:137:GLU:HG3	1.97	0.45
1:B:154:LYS:NZ	1:B:243:GLU:OE2	2.33	0.45
1:B:79:LYS:NZ	6:B:508:HOH:O	2.49	0.45
1:A:224:GLU:O	1:A:240:PRO:HA	2.17	0.45
1:B:196:LYS:HA	1:B:199:MET:HE2	1.99	0.45
1:B:219:ASN:O	1:B:220:HIS:HB2	2.17	0.45



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Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	Clash overlap (Å)
1:B:122:ILE:HB	1:B:253:ASP:HB3	1.98	0.45
1:B:201:SER:OG	1:B:202:SER:N	2.51	0.44
1:A:87:LYS:NZ	1:A:253:ASP:OD2	2.40	0.43
3:A:402:TLA:O2	3:A:402:TLA:O4	2.27	0.42
1:A:320:GLN:HG2	1:A:322:ASP:OD1	2.20	0.42
1:A:44:LYS:O	1:A:47:VAL:HB	2.19	0.42
1:B:132:GLY:O	1:B:135:ARG:HB3	2.19	0.42
1:B:49:PRO:HA	1:B:64:GLY:HA3	2.00	0.42
1:B:87:LYS:NZ	1:B:253:ASP:OD2	2.48	0.42
1:B:333:ASN:OD1	1:B:335:VAL:HB	2.21	0.41
1:B:135:ARG:HE	1:B:221:GLU:HG3	1.86	0.41
1:B:191:HIS:CD2	1:B:193:ALA:HB3	2.55	0.41
1:B:328:MET:HB3	1:B:333:ASN:ND2	2.36	0.41
1:A:278:SER:HB3	1:A:287:ALA:O	2.21	0.40
1:A:183:TYR:CE2	1:A:185:LYS:HB2	2.56	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	entiles
1	A	$344/349 \ (99\%)$	327 (95%)	16 (5%)	1 (0%)	41	55
1	В	341/349 (98%)	323 (95%)	14 (4%)	4 (1%)	13	19
All	All	$685/698 \; (98\%)$	650 (95%)	30 (4%)	5 (1%)	22	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	345	LYS
1	В	131	GLU
1	В	218	ASP



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Mol	Chain	Res	Type
1	A	189	SER
1	В	189	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	293/296 (99%)	284 (97%)	9 (3%)	40 60		
1	В	290/296 (98%)	280 (97%)	10 (3%)	37 56		
All	All	583/592 (98%)	564 (97%)	19 (3%)	38 57		

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	59	LEU
1	A	62	VAL
1	A	192	GLU
1	A	200	ASN
1	A	218	ASP
1	A	237	SER
1	A	258	GLU
1	A	341	ARG
1	В	105	THR
1	В	111	SER
1	В	134	GLU
1	В	164	SER
1	В	200	ASN
1	В	237	SER
1	В	306	GLN
1	В	329	VAL
1	В	335	VAL
1	В	347	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:



Mol	Chain	${f Res}$	\mathbf{Type}
1	В	70	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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 Ch		Chain	nain Res		В	Bond lengths			Bond angles			
MIOI	Type	Chain	nes	nes	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OXM	В	402	-	2,5,5	0.43	0	2,6,6	1.17	0		
3	TLA	A	402	-	3,9,9	0.73	0	6,12,12	1.08	1 (16%)		
5	ACT	В	403	-	1,3,3	6.30	1 (100%)	0,3,3	0.00	-		
2	FAD	A	401	-	51,58,58	1.46	7 (13%)	60,89,89	2.55	14 (23%)		
4	OXM	A	403	-	2,5,5	0.57	0	2,6,6	1.38	0		
2	FAD	В	401	-	51,58,58	1.43	6 (11%)	60,89,89	2.55	14 (23%)		

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	FAD	A	401	-	-	9/30/50/50	0/6/6/6
3	TLA	A	402	-	-	4/4/12/12	-
4	OXM	В	402	_	-	0/0/4/4	-
2	FAD	В	401	_	-	8/30/50/50	0/6/6/6
4	OXM	A	403	-	-	0/0/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
5	В	403	ACT	СН3-С	6.30	1.56	1.48
2	В	401	FAD	C4X-C10	5.89	1.44	1.38
2	A	401	FAD	C4X-C10	5.89	1.44	1.38
2	A	401	FAD	C4X-N5	-4.16	1.27	1.33
2	В	401	FAD	C9A-N10	3.49	1.43	1.38
2	A	401	FAD	C9A-N10	3.32	1.43	1.38
2	В	401	FAD	C4X-N5	-3.21	1.28	1.33
2	В	401	FAD	C1'-N10	3.13	1.51	1.48
2	A	401	FAD	C4-N3	2.72	1.37	1.33
2	A	401	FAD	C4-C4X	2.67	1.46	1.41
2	В	401	FAD	C4-C4X	2.65	1.45	1.41
2	A	401	FAD	C1'-N10	2.59	1.50	1.48
2	В	401	FAD	C10-N1	-2.24	1.30	1.33
2	A	401	FAD	C4'-C3'	2.15	1.57	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
2	В	401	FAD	C4-N3-C2	12.80	125.95	115.14
2	A	401	FAD	C4-N3-C2	12.54	125.73	115.14
2	В	401	FAD	C4X-C4-N3	-7.05	113.79	123.43
2	A	401	FAD	C4X-C4-N3	-6.98	113.88	123.43
2	A	401	FAD	C5'-C4'-C3'	6.18	124.15	112.20
2	В	401	FAD	C5'-C4'-C3'	6.03	123.85	112.20
2	A	401	FAD	C10-C4X-N5	5.30	124.92	121.26
2	В	401	FAD	C10-C4X-N5	5.06	124.76	121.26
2	A	401	FAD	C1'-N10-C9A	4.99	122.22	118.29
2	В	401	FAD	C1'-N10-C9A	4.81	122.08	118.29
2	A	401	FAD	C4-C4X-C10	-3.38	117.71	119.95
2	В	401	FAD	C4-C4X-C10	-3.34	117.74	119.95
2	В	401	FAD	O4'-C4'-C5'	-3.11	102.92	109.92
2	A	401	FAD	C4X-C10-N10	-2.94	117.28	120.30
2	В	401	FAD	C9A-N10-C10	-2.86	118.16	121.91



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
2	A	401	FAD	C9A-N10-C10	-2.83	118.21	121.91
2	A	401	FAD	O4'-C4'-C5'	-2.81	103.60	109.92
2	В	401	FAD	C4X-C10-N10	-2.73	117.50	120.30
2	В	401	FAD	O3'-C3'-C2'	-2.71	102.27	108.81
2	В	401	FAD	C1'-N10-C10	-2.61	116.07	118.41
2	В	401	FAD	C5A-C6A-N6A	2.33	123.90	120.35
2	A	401	FAD	O2'-C2'-C3'	-2.31	103.48	109.10
2	A	401	FAD	O2P-P-O5'	2.30	118.41	107.75
2	В	401	FAD	C6-C5X-N5	-2.29	116.53	119.05
2	A	401	FAD	C5A-C6A-N6A	2.18	123.67	120.35
2	A	401	FAD	C6-C5X-N5	-2.18	116.65	119.05
2	A	401	FAD	C1'-N10-C10	-2.14	116.49	118.41
2	В	401	FAD	O2P-P-O5'	2.13	117.64	107.75
3	A	402	TLA	C4-C3-C2	-2.04	108.72	113.11

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	TLA	C1-C2-C3-C4
2	A	401	FAD	N10-C1'-C2'-O2'
2	A	401	FAD	N10-C1'-C2'-C3'
2	A	401	FAD	C2'-C3'-C4'-O4'
2	A	401	FAD	C2'-C3'-C4'-C5'
2	A	401	FAD	O3'-C3'-C4'-O4'
2	A	401	FAD	O3'-C3'-C4'-C5'
2	В	401	FAD	N10-C1'-C2'-O2'
2	В	401	FAD	N10-C1'-C2'-C3'
2	В	401	FAD	C2'-C3'-C4'-O4'
2	В	401	FAD	C2'-C3'-C4'-C5'
2	В	401	FAD	O3'-C3'-C4'-O4'
2	В	401	FAD	O3'-C3'-C4'-C5'
2	В	401	FAD	O4B-C4B-C5B-O5B
3	A	402	TLA	O2-C2-C3-O3
2	A	401	FAD	C3'-C4'-C5'-O5'
2	A	401	FAD	PA-O3P-P-O5'
3	A	402	TLA	O2-C2-C3-C4
2	A	401	FAD	O4B-C4B-C5B-O5B
2	В	401	FAD	C3B-C4B-C5B-O5B
3	A	402	TLA	C1-C2-C3-O3

There are no ring outliers.

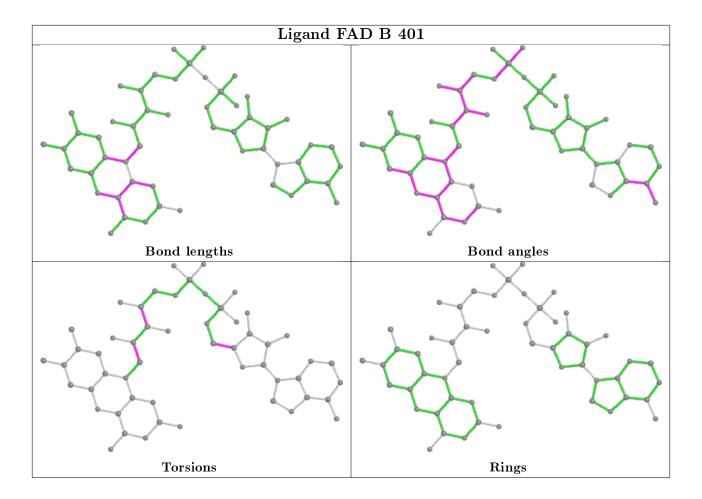


0			•	1 1	•	0	1 /	1 1
-3	monomers	are	invo	lved	ın	3 s	hort	contacts:

Mol	Chain	${ m Res}$	Type	Clashes	Symm-Clashes
3	A	402	TLA	1	0
2	A	401	FAD	1	0
2	В	401	FAD	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 $>$	$\#\mathrm{RSRZ}{>}2$		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	346/349 (99%)	-0.19	17 (4%) 29	28	17, 35, 83, 108	0
1	В	343/349 (98%)	-0.10	23 (6%) 1	7 16	18, 35, 84, 108	0
All	All	689/698 (98%)	-0.15	40 (5%) 23	22	17, 35, 84, 108	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	195	VAL	8.1
1	A	191	HIS	7.4
1	В	189	SER	7.3
1	В	191	HIS	6.5
1	В	193	ALA	6.2
1	В	194	GLN	5.3
1	В	186	GLU	5.1
1	A	219	ASN	4.9
1	A	192	GLU	4.8
1	В	192	GLU	4.5
1	A	187	GLU	4.4
1	В	187	GLU	4.4
1	В	188	LEU	4.3
1	A	199	MET	4.2
1	A	189	SER	4.1
1	В	199	MET	4.1
1	В	163	ASN	3.8
1	В	190	GLY	3.7
1	A	194	GLN	3.6
1	A	190	GLY	3.5
1	В	197	GLN	3.4
1	В	196	LYS	3.3
1	A	186	GLU	3.1
1	В	232	GLU	3.1



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Mol	Chain	Res	Type	RSRZ
1	В	220	HIS	3.1
1	В	183	TYR	3.1
1	A	188	LEU	3.1
1	В	201	SER	3.1
1	A	218	ASP	2.9
1	A	163	ASN	2.8
1	A	220	HIS	2.6
1	A	193	ALA	2.6
1	В	198	LEU	2.4
1	В	219	ASN	2.3
1	В	200	ASN	2.3
1	В	132	GLY	2.2
1	A	349	LYS	2.2
1	A	198	LEU	2.1
1	A	231	HIS	2.1
1	В	233	THR	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 monosaccharides in this entry.

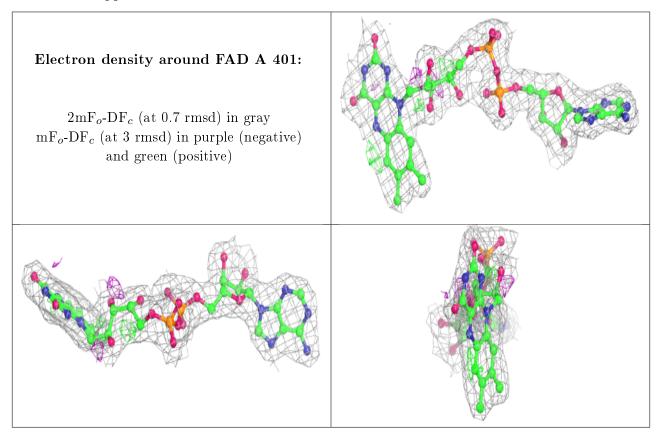
6.4 Ligands (i)

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.

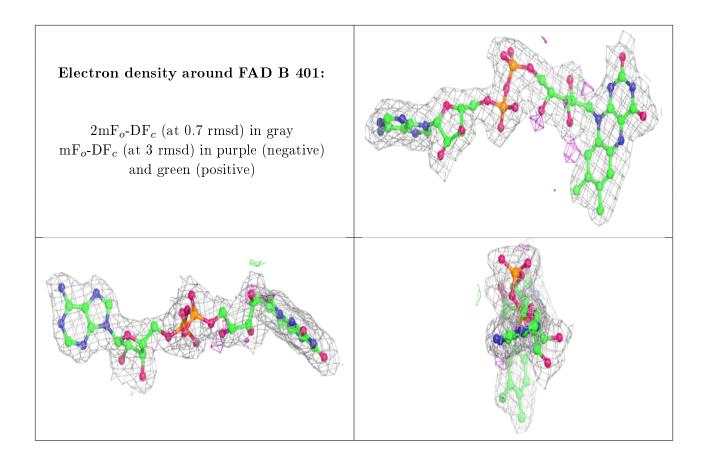
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	OXM	В	402	6/6	0.88	0.16	43,49,51,51	0
4	OXM	A	403	6/6	0.90	0.11	42,46,48,53	0
3	TLA	A	402	10/10	0.91	0.30	49,54,58,64	0
5	ACT	В	403	4/4	0.92	0.17	35,42,48,56	0
2	FAD	A	401	53/53	0.97	0.12	18,24,30,32	0
2	FAD	В	401	53/53	0.97	0.13	16,24,28,32	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.

