

wwPDB X-ray Structure Validation Summary Report (i)

Dec 2, 2023 - 02:57 pm GMT

PDB ID : 2IVE

Title: Structure of protoporphyrinogen oxidase from Myxococcus xanthus

Authors: Corradi, H.R.; Corrigall, A.V.; Boix, E.; Mohan, C.G.; Sturrock, E.D.; Meiss-

ner, P.N.; Acharya, K.R.

Deposited on : 2006-06-13

Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

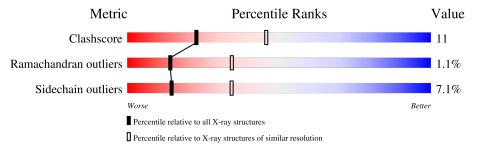
Validation Pipeline (wwPDB-VP) : 2.36

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 2.70 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 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 <=5%

Mol	Chain	Length	Quality of chain	
1	A	478	78%	12% • • 6%
1	В	478	81%	11% • 6%

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:

\mathbf{Mol}	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TWN	A	4002	-	-	X	-



2 Entry composition (i)

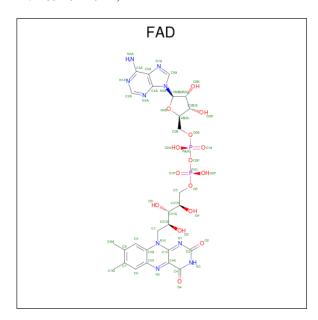
There are 5 unique types of molecules in this entry. The entry contains 7011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTOPORPHYRINOGEN OXIDASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	451	Total 3326	C 2093	N 627	O 600	S 6	34	0	0
1	В	450	Total 3322	C 2090	N 628	O 598	S 6	29	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	С	N	О	Р	0	0
	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	U

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

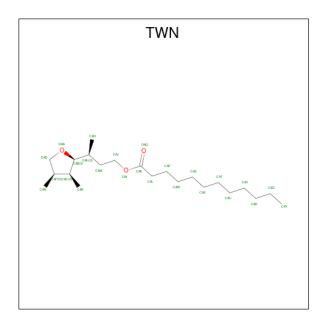




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	В	1	Total C O 6 3 3	0	0
3	В	1	Total C O 6 3 3	0	0
3	В	1	Total C O 6 3 3	0	0

• Molecule 4 is (3S)-3-[(2S,3S,4R)-3,4-DIMETHYLTETRAHYDROFURAN-2-YL]BUTYL LAURATE (three-letter code: TWN) (formula: $C_{22}H_{42}O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 25 22 3	0	0
4	В	1	Total C O 25 22 3	0	0
4	В	1	Total C O 25 22 3	0	0

• Molecule 5 is water.

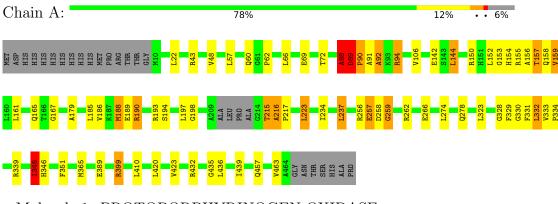
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	74	Total O 74 74	0	0
5	В	72	Total O 72 72	0	0



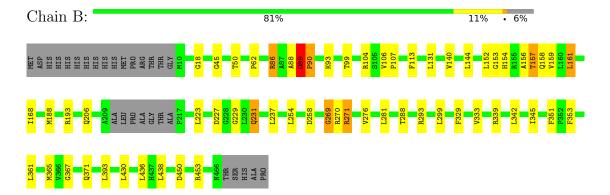
3 Residue-property plots (i)

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. 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. 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: PROTOPORPHYRINOGEN OXIDASE



• Molecule 1: PROTOPORPHYRINOGEN OXIDASE





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants	148.57Å 148.57Å 132.75Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.33 - 2.70	Depositor
Resolution (A)	74.28 - 2.70	EDS
% Data completeness	99.9 (74.33-2.70)	Depositor
(in resolution range)	99.9 (74.28-2.70)	EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.29 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D.	0.247 , 0.287	Depositor
R, R_{free}	(Not available) , (Not available)	DCC
R_{free} test set	857 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 1.9	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.52	EDS
Total number of atoms	7011	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.12% 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: GOL, TWN, FAD

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		nd lengths	Bond angles		
Mol Chain		RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.37	1/3384 (0.0%)	0.58	2/4593 (0.0%)	
1	В	0.37	1/3380 (0.0%)	0.57	3/4586 (0.1%)	
All	All	0.37	$2/6764 \ (0.0\%)$	0.57	5/9179 (0.1%)	

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	4
1	В	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
1	A	262	ARG	CD-NE	6.97	1.58	1.46
1	В	93	LYS	CB-CG	-5.40	1.38	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	206	GLN	CG-CD-OE1	-6.10	109.39	121.60
1	A	259	GLY	N-CA-C	-5.56	99.20	113.10
1	В	93	LYS	CA-CB-CG	5.53	125.56	113.40
1	В	89	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	89	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.



5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	345	ILE	Peptide
1	A	88	ALA	Peptide
1	A	89	ASP	Peptide
1	A	92	ALA	Peptide
1	В	89	ASP	Peptide

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	3326	0	3382	83	0
1	В	3322	0	3379	53	0
2	A	53	0	31	2	0
2	В	53	0	31	3	0
3	A	18	0	24	2	0
3	В	18	0	24	1	0
4	A	25	0	42	21	0
4	В	50	0	83	17	0
5	A	74	0	0	0	0
5	В	72	0	0	0	0
All	All	7011	0	6996	157	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 11.

The worst 5 of 157 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:92:ALA:CB	1:A:328:GLY:HA2	1.43	1.45
1:A:92:ALA:HB3	1:A:328:GLY:CA	1.47	1.43
4:B:4003:TWN:HAK3	4:B:4003:TWN:CAO	1.55	1.31
4:B:4003:TWN:HAO1	4:B:4003:TWN:CAK	1.58	1.30
4:A:4002:TWN:HAX2	4:A:4002:TWN:CAR	1.50	1.28

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	Pe	rce	entiles
1	A	447/478 (94%)	423 (95%)	17 (4%)	7 (2%)		9	24
1	В	446/478 (93%)	426 (96%)	17 (4%)	3 (1%)	4	22	46
All	All	893/956 (93%)	849 (95%)	34 (4%)	10 (1%)		14	34

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	215	THR
1	A	216	ALA
1	В	89	ASP
1	В	90	PRO

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	319/344 (93%)	294 (92%)	25 (8%)	12 29		
1	В	319/344 (93%)	299 (94%)	20 (6%)	18 40		
All	All	638/688 (93%)	593 (93%)	45 (7%)	14 34		

5 of 45 residues with a non-rotameric sidechain are listed below:

\mathbf{Mol}	Chain	Res	\mathbf{Type}
1	В	140	VAL

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	В	237	LEU
1	В	144	LEU
1	В	161	LEU
1	В	271	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	60	GLN
1	В	154	HIS
1	В	457	GLN
1	A	346	HIS
1	A	416	ASN

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)

11 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	Tuno	Chain	Res	Link	Bo	ond leng	ths	Е	ond ang	gles	
MIOI	Type	Chain	rtes	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	3003	-	5,5,5	0.41	0	5,5,5	0.23	0	
2	FAD	В	2114	-	53,58,58	1.16	4 (7%)	68,89,89	1.36	10 (14%)	
3	GOL	В	3005	-	5,5,5	0.35	0	5,5,5	0.28	0	
4	TWN	В	4003	-	25,25,25	0.58	0	25,30,30	1.56	6 (24%)	
3	GOL	В	3007	-	5,5,5	0.39	0	5,5,5	0.22	0	
4	TWN	A	4002	-	25,25,25	0.63	0	25,30,30	1.16	2 (8%)	
3	GOL	A	3001	-	5,5,5	0.33	0	5,5,5	0.36	0	
2	FAD	A	2114	-	53,58,58	1.17	4 (7%)	68,89,89	1.38	9 (13%)	
3	GOL	A	3002	-	5,5,5	0.37	0	5,5,5	0.21	0	
3	GOL	В	3006	-	5,5,5	0.35	0	5,5,5	0.27	0	
4	TWN	В	4001	-	25,25,25	0.69	1 (4%)	25,30,30	1.34	6 (24%)	

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	GOL	A	3003	-	-	0/4/4/4	-
2	FAD	В	2114	-	-	3/30/50/50	0/6/6/6
3	GOL	В	3005	-	-	3/4/4/4	-
4	TWN	В	4003	-	-	11/21/34/34	0/1/1/1
3	GOL	В	3007	-	-	2/4/4/4	-
4	TWN	A	4002	-	-	12/21/34/34	0/1/1/1
3	GOL	A	3001	-	-	2/4/4/4	-
2	FAD	A	2114	-	-	4/30/50/50	0/6/6/6
3	GOL	A	3002	-	-	2/4/4/4	-
3	GOL	В	3006	-	-	2/4/4/4	-
4	TWN	В	4001	-	-	12/21/34/34	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
2	A	2114	FAD	C4X-N5	4.26	1.39	1.30
2	В	2114	FAD	C4X-N5	4.18	1.38	1.30
2	A	2114	FAD	C2A-N3A	4.15	1.38	1.32
2	В	2114	FAD	C2A-N3A	4.10	1.38	1.32
2	A	2114	FAD	C10-N1	2.89	1.39	1.33



The worst 5	of	33	bond	angle	outliers	are	listed	below:
1110 110100 0	01	\mathbf{O}	OIIG	WII SIC	Cathere	COL C	IID CCC	OCIO III.

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	2114	FAD	N3A-C2A-N1A	-5.57	119.97	128.68
2	В	2114	FAD	N3A-C2A-N1A	-5.57	119.97	128.68
4	В	4003	TWN	OAA-CAB-CAH	3.62	117.27	109.37
4	A	4002	TWN	OAI-CAE-CAL	3.24	122.07	111.91
2	В	2114	FAD	P-O3P-PA	-3.03	122.41	132.83

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2114	FAD	N10-C1'-C2'-O2'
2	A	2114	FAD	N10-C1'-C2'-C3'
2	В	2114	FAD	N10-C1'-C2'-O2'
3	A	3002	GOL	C1-C2-C3-O3
3	В	3005	GOL	O1-C1-C2-C3

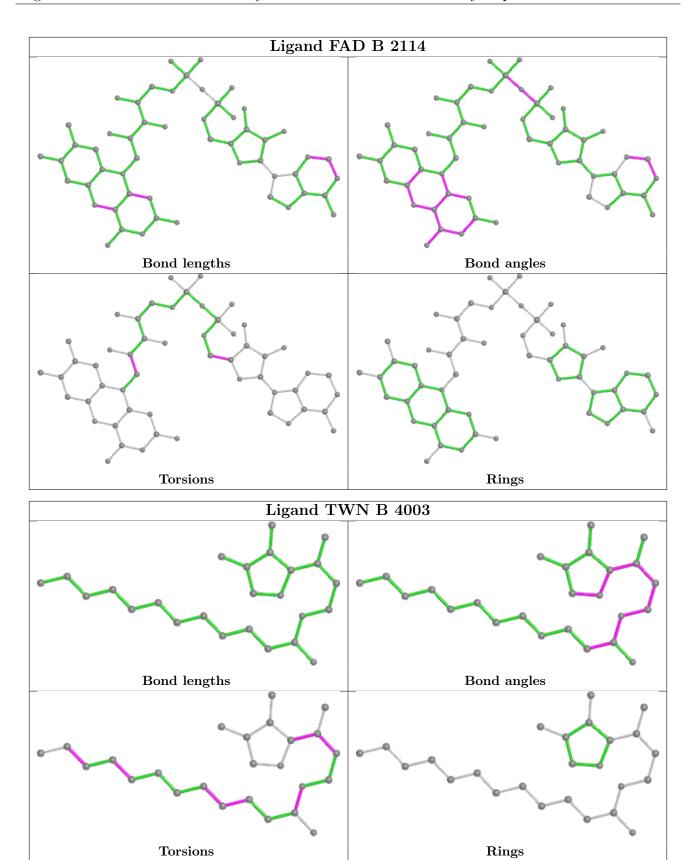
There are no ring outliers.

7 monomers are involved in 43 short contacts:

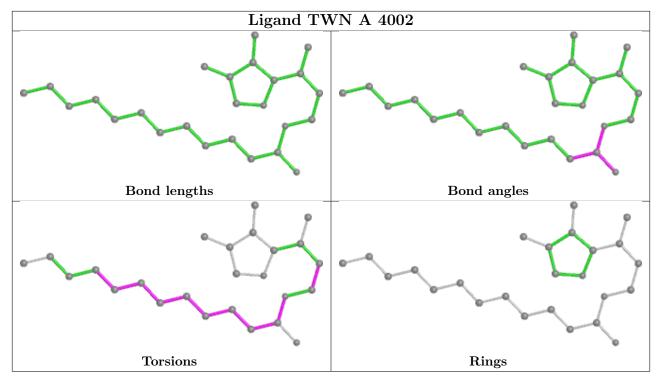
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	2114	FAD	3	0
4	В	4003	TWN	14	0
3	В	3007	GOL	1	0
4	A	4002	TWN	21	0
2	A	2114	FAD	2	0
3	A	3002	GOL	2	0
4	В	4001	TWN	3	0

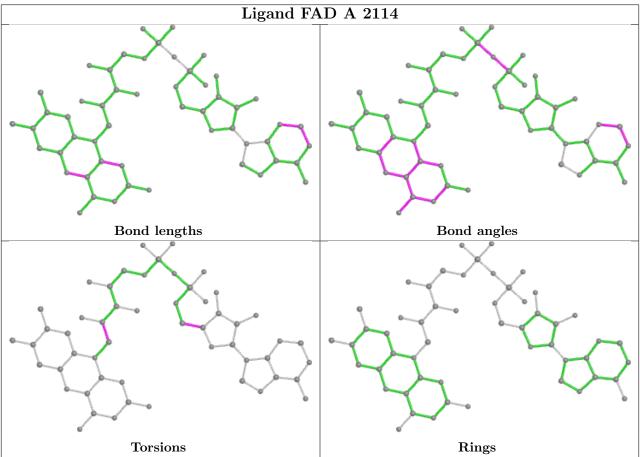
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



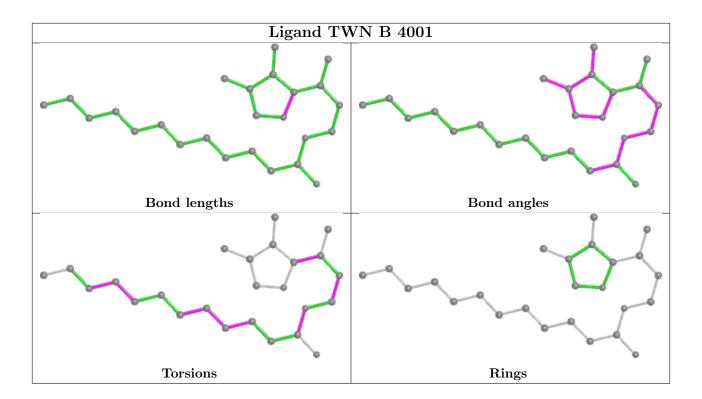












5.7 Other polymers (i)

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

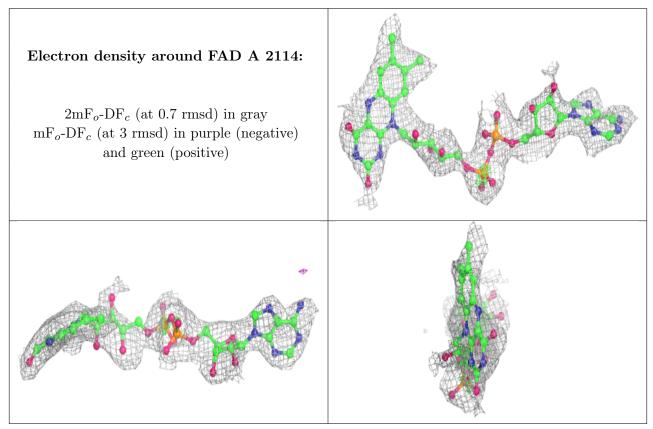
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

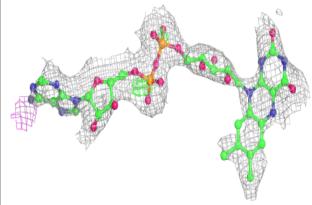
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

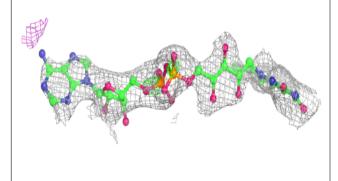


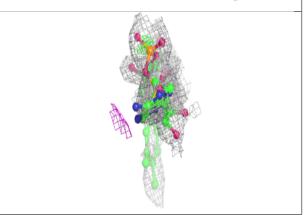


Electron density around FAD B 2114:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

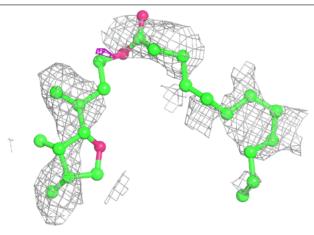


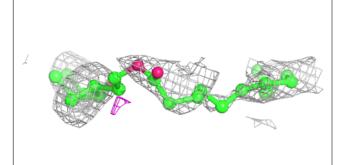


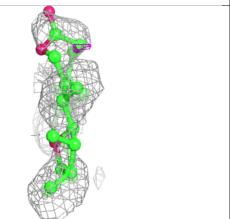


Electron density around TWN A 4002:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



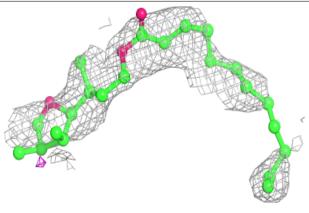


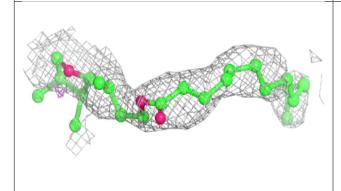


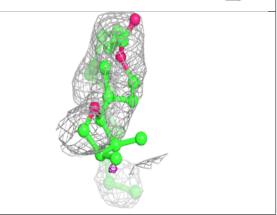


Electron density around TWN B 4001:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

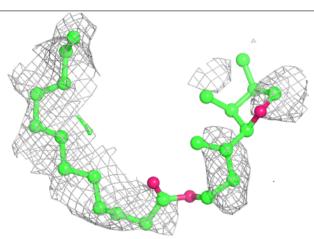


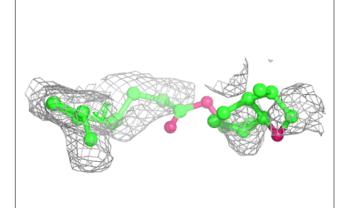


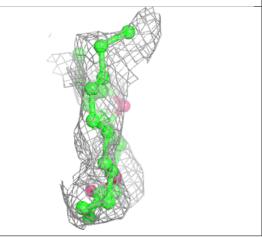


Electron density around TWN B 4003:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

