



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:43 PM UTC

PDB ID : 4USR / pdb_00004usr
Title : Structure of flavin-containing monooxygenase from *Pseudomonas stutzeri* NF13
Authors : Jensen, C.N.; Ali, S.T.; Allen, M.J.; Grogan, G.
Deposited on : 2014-07-11
Resolution : 1.83 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

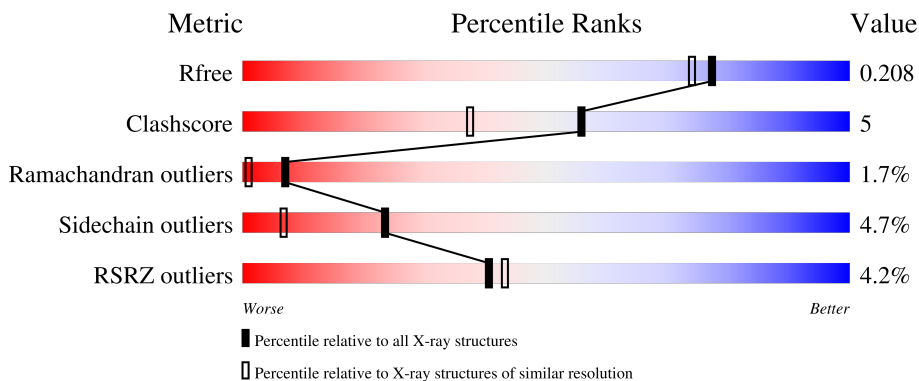
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

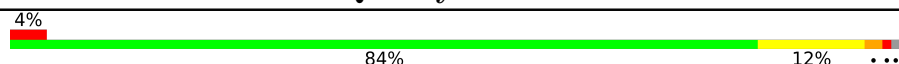
The reported resolution of this entry is 1.83 Å.

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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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 $\leq 5\%$. 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	361	

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

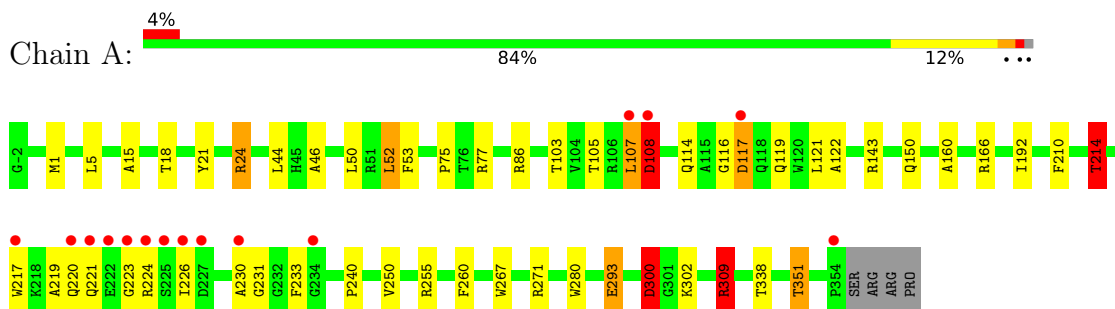
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	211	Total O 211 211	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: MONOOXYGENASE



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	63.56Å 63.56Å 189.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.94 – 1.83 35.94 – 1.83	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.94-1.83) 99.9 (35.94-1.83)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 1.76Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.162 , 0.204 0.175 , 0.208	Depositor DCC
R_{free} test set	2275 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtrriage
Anisotropy	0.514	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3048	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: FAD, GOL

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	1.33	4/2882 (0.1%)	1.23	23/3947 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105[A]	THR	CA-C	12.37	1.67	1.52
1	A	105[B]	THR	CA-C	12.37	1.67	1.52
1	A	108	ASP	CA-C	6.67	1.61	1.52
1	A	260	PHE	N-CA	-5.78	1.38	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ASP	N-CA-C	-8.70	92.27	110.80
1	A	108	ASP	CB-CA-C	8.23	126.79	110.42
1	A	351	THR	CB-CA-C	-7.69	95.38	109.54
1	A	351	THR	N-CA-CB	7.12	120.42	110.17
1	A	86	ARG	NE-CZ-NH2	-6.18	113.63	119.20
1	A	86	ARG	NE-CZ-NH1	6.10	127.60	121.50
1	A	293	GLU	CA-CB-CG	-6.03	102.05	114.10
1	A	116	GLY	CA-C-N	5.91	129.29	120.31
1	A	116	GLY	C-N-CA	5.91	129.29	120.31
1	A	351	THR	OG1-CB-CG2	5.75	120.81	109.30
1	A	105[A]	THR	CA-C-O	5.73	126.55	120.36
1	A	105[B]	THR	CA-C-O	5.73	126.55	120.36
1	A	300	ASP	N-CA-C	5.65	122.83	110.80
1	A	214	THR	OG1-CB-CG2	5.48	120.27	109.30
1	A	300	ASP	CB-CA-C	-5.48	99.51	110.42
1	A	117	ASP	N-CA-C	5.47	118.17	111.82
1	A	117	ASP	CB-CA-C	-5.43	100.25	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ALA	CA-C-N	-5.29	114.37	119.87
1	A	160	ALA	C-N-CA	-5.29	114.37	119.87
1	A	309	ARG	CD-NE-CZ	5.21	131.69	124.40
1	A	309	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	A	240	PRO	CA-C-N	-5.03	113.86	119.19
1	A	240	PRO	C-N-CA	-5.03	113.86	119.19

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	2778	0	2717	26	0
2	A	53	0	31	0	0
3	A	6	0	8	0	0
4	A	211	0	0	5	0
All	All	3048	0	2756	26	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 (26) 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:309:ARG:HD2	4:A:2186:HOH:O	1.58	1.01
1:A:300:ASP:HB3	1:A:302:LYS:H	1.49	0.76
1:A:117:ASP:HB2	4:A:2094:HOH:O	1.86	0.74
1:A:107:LEU:C	1:A:108:ASP:O	2.23	0.73
1:A:150:GLN:HE21	1:A:280:TRP:HE1	1.35	0.72
1:A:21:TYR:O	1:A:24:ARG:HG3	1.95	0.66
1:A:309:ARG:CD	4:A:2186:HOH:O	2.31	0.65
1:A:44:LEU:O	1:A:77:ARG:NH2	2.31	0.63
1:A:210:PHE:O	1:A:214:THR:HG23	2.01	0.60
1:A:219:ALA:O	1:A:224:ARG:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:THR:HA	1:A:217:TRP:CD1	2.48	0.49
1:A:143:ARG:HH11	1:A:150:GLN:HE22	1.61	0.49
1:A:46:ALA:HB1	1:A:50:LEU:HD13	1.95	0.48
1:A:114[B]:GLN:HG3	1:A:119:GLN:HG2	1.96	0.48
1:A:293:GLU:HG3	4:A:2089:HOH:O	2.13	0.48
1:A:143:ARG:HH11	1:A:150:GLN:NE2	2.12	0.47
1:A:52:LEU:HD22	1:A:75:PRO:HB2	1.97	0.47
1:A:338:THR:HG23	4:A:2201:HOH:O	2.15	0.46
1:A:1:MET:HE3	1:A:1:MET:HB3	1.85	0.46
1:A:46:ALA:HB3	1:A:77:ARG:HG3	1.98	0.46
1:A:267:TRP:HB2	1:A:271:ARG:HB2	2.00	0.42
1:A:5:LEU:O	1:A:122:ALA:HA	2.19	0.42
1:A:255:ARG:NE	1:A:255:ARG:HA	2.36	0.41
1:A:231:GLY:HA3	1:A:233:PHE:CE2	2.56	0.40
1:A:15:ALA:O	1:A:18[B]:THR:HG22	2.21	0.40
1:A:50:LEU:C	1:A:50:LEU:HD23	2.46	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	Percentiles
1	A	364/361 (101%)	345 (95%)	13 (4%)	6 (2%)	7 1

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	A	220	GLN
1	A	223	GLY
1	A	108	ASP
1	A	230	ALA

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Mol	Chain	Res	Type
1	A	226	ILE

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	285/291 (98%)	271 (95%)	14 (5%)	22 6

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	52	LEU
1	A	53	PHE
1	A	103[A]	THR
1	A	103[B]	THR
1	A	107	LEU
1	A	121	LEU
1	A	166	ARG
1	A	192	ILE
1	A	214	THR
1	A	250	VAL
1	A	300	ASP
1	A	309	ARG
1	A	351	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	150	GLN
1	A	194	GLN
1	A	274	ASN
1	A	315	ASN
1	A	348	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 oligosaccharides 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	1355	-	58,58,58	1.47	7 (12%)	85,89,89	1.61	14 (16%)
3	GOL	A	1356	-	5,5,5	1.06	0	5,5,5	1.19	1 (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	Torsions	Rings
2	FAD	A	1355	-	-	1/34/50/50	0/6/6/6
3	GOL	A	1356	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1355	FAD	C9A-C5X	4.00	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1355	FAD	C1'-C2'	-3.89	1.47	1.52
2	A	1355	FAD	C4X-N5	3.46	1.38	1.30
2	A	1355	FAD	P-O3P	3.31	1.63	1.59
2	A	1355	FAD	C4A-N9A	-2.96	1.31	1.37
2	A	1355	FAD	O4-C4	2.72	1.28	1.23
2	A	1355	FAD	C8A-N9A	-2.10	1.34	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1355	FAD	C5A-C4A-N3A	-4.87	120.01	126.72
2	A	1355	FAD	C2'-C1'-N10	4.57	131.78	110.20
2	A	1355	FAD	O2-C2-N1	-3.98	115.19	121.80
2	A	1355	FAD	N3A-C2A-N1A	-3.56	123.20	128.58
2	A	1355	FAD	N3A-C4A-N9A	3.34	132.85	127.17
2	A	1355	FAD	C2A-N3A-C4A	2.90	118.91	111.83
2	A	1355	FAD	O4-C4-C4X	-2.89	118.91	126.53
2	A	1355	FAD	C4A-C5A-N7A	-2.80	107.38	110.58
2	A	1355	FAD	C4'-C3'-C2'	-2.66	109.14	113.57
2	A	1355	FAD	O2-C2-N3	2.40	123.19	118.58
2	A	1355	FAD	C9A-C5X-N5	-2.35	119.96	122.45
2	A	1355	FAD	C4-C4X-N5	2.24	121.30	118.21
2	A	1355	FAD	C4A-N9A-C8A	2.20	108.05	105.74
2	A	1355	FAD	O2A-PA-O1A	2.05	121.97	112.44
3	A	1356	GOL	C3-C2-C1	-2.04	104.32	111.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

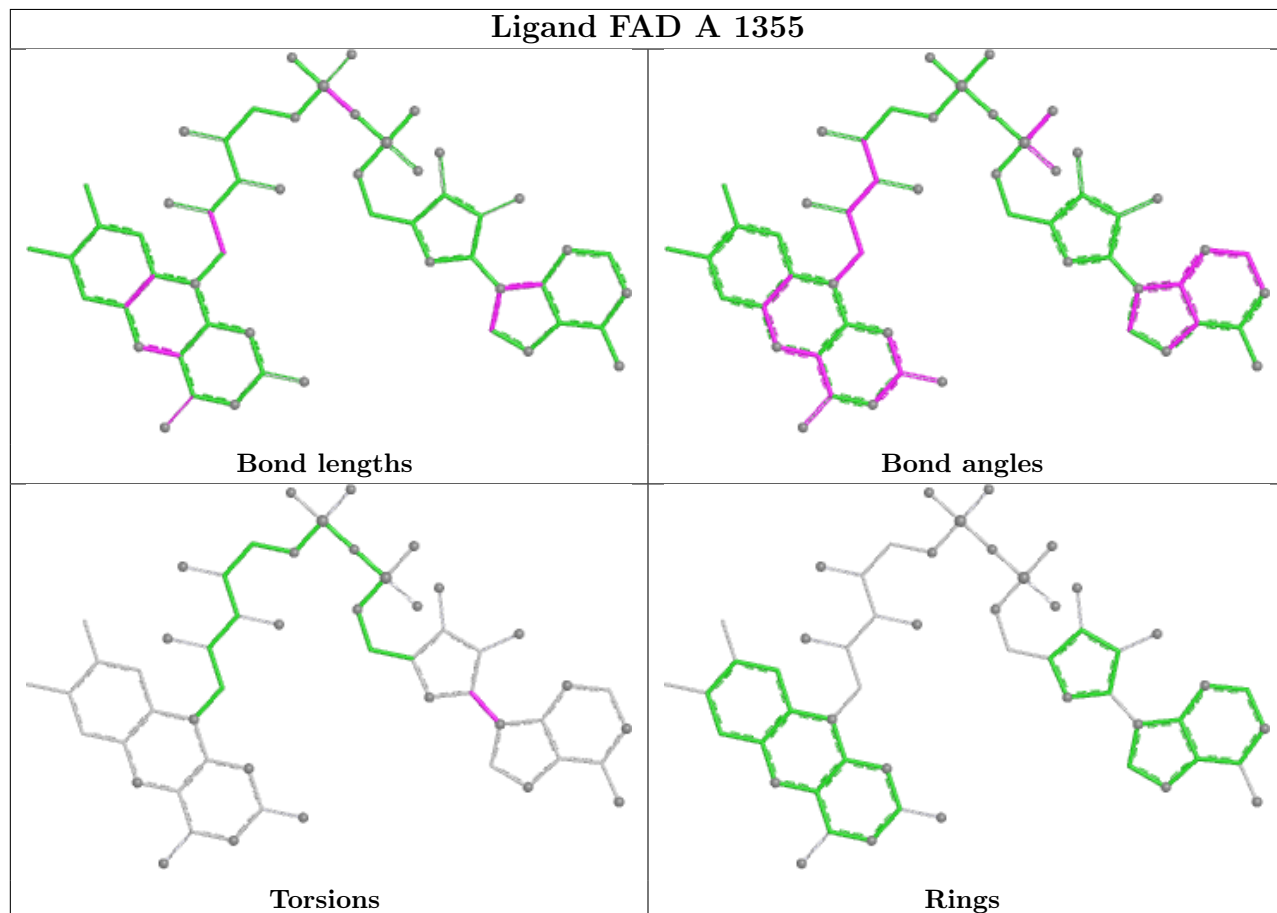
Mol	Chain	Res	Type	Atoms
2	A	1355	FAD	C2B-C1B-N9A-C8A

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 than 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, 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	357/361 (98%)	-0.19	15 (4%) 40 43	8, 17, 36, 74	9 (2%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	ILE	5.1
1	A	225	SER	4.7
1	A	224	ARG	4.1
1	A	227	ASP	4.0
1	A	223	GLY	3.9
1	A	222	GLU	3.2
1	A	234	GLY	2.7
1	A	220	GLN	2.7
1	A	221	GLN	2.4
1	A	354	PRO	2.3
1	A	117	ASP	2.3
1	A	217	TRP	2.2
1	A	108	ASP	2.2
1	A	107	LEU	2.2
1	A	230	ALA	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](#)

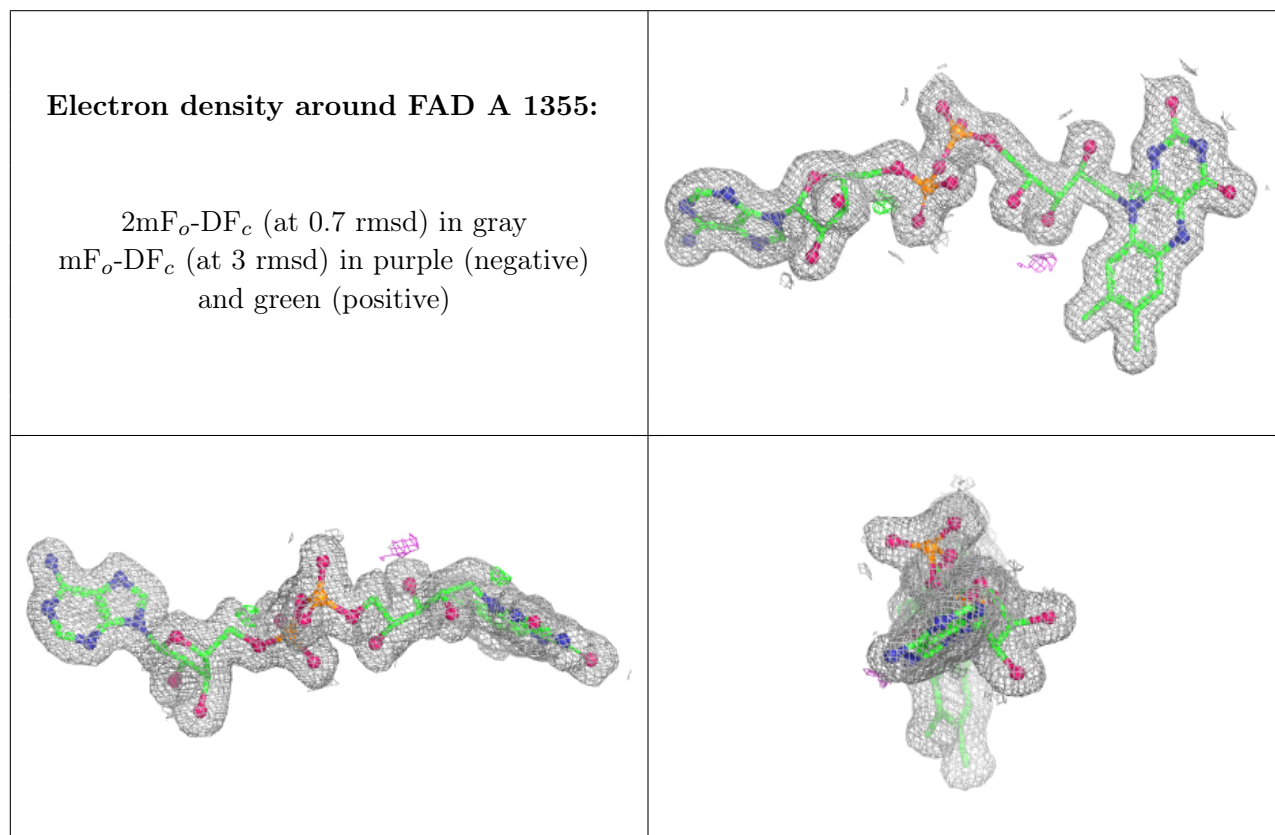
There are no oligosaccharides in this entry.

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
3	GOL	A	1356	6/6	0.91	0.10	29,30,32,33	0
2	FAD	A	1355	53/53	0.98	0.04	10,11,14,17	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.