



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2024 – 06:07 PM JST

PDB ID : 8JZ3
Title : Crystal structure of AetF in complex with FAD and L-tryptophan
Authors : Li, H.; Dai, L.; Chen, C.-C.; Guo, R.-T.
Deposited on : 2023-07-04
Resolution : 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 ⓘ 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 : 4.02b-467
Mogul : 1.8.5 (274361), 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 : 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

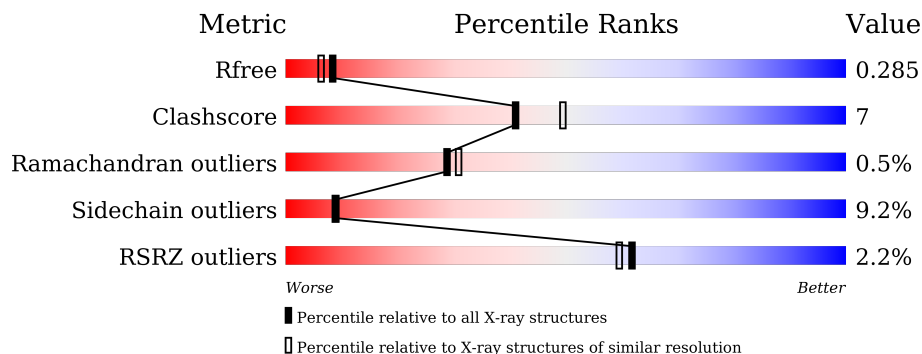
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
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 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	679	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5578 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.

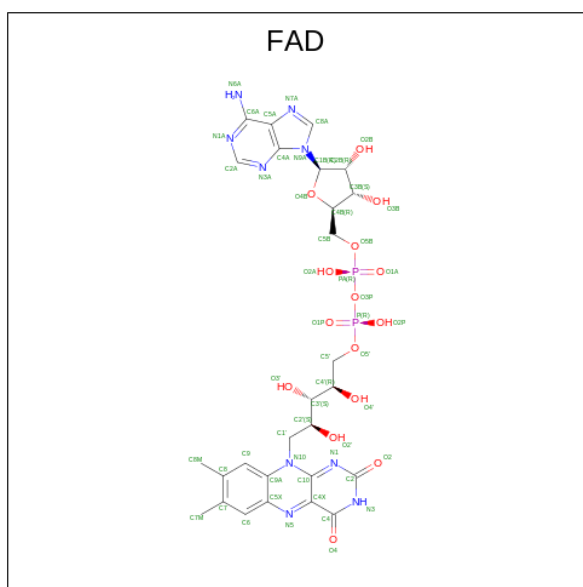
- Molecule 1 is a protein called AetF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	629	5202	3342	880	965	15	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

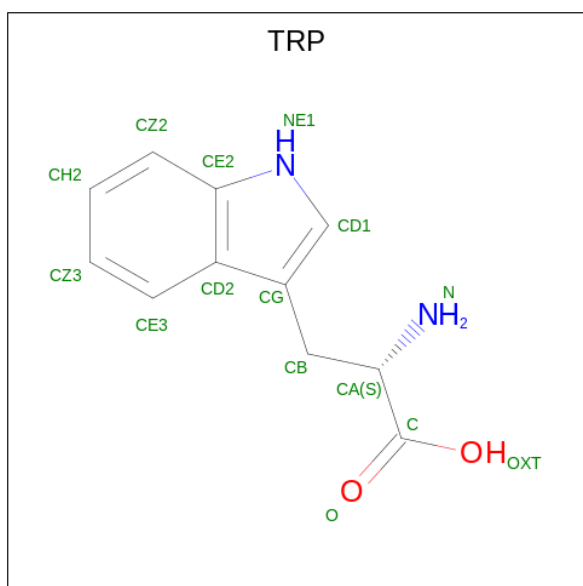
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP A0A861B9Z9
A	-9	ALA	-	expression tag	UNP A0A861B9Z9
A	-8	GLY	-	expression tag	UNP A0A861B9Z9
A	-7	ALA	-	expression tag	UNP A0A861B9Z9
A	-6	GLY	-	expression tag	UNP A0A861B9Z9
A	-5	ALA	-	expression tag	UNP A0A861B9Z9
A	-4	GLY	-	expression tag	UNP A0A861B9Z9
A	-3	ALA	-	expression tag	UNP A0A861B9Z9
A	-2	GLY	-	expression tag	UNP A0A861B9Z9
A	-1	ALA	-	expression tag	UNP A0A861B9Z9
A	0	GLY	-	expression tag	UNP A0A861B9Z9

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	11	2	2	0	0
3	A	1	15	11	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	293	Total 293	O 293	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.24Å 74.86Å 143.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.16 – 2.20 33.16 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.16-2.20) 99.6 (33.16-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.206 , 0.285 0.210 , 0.285	Depositor DCC
R_{free} test set	1584 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtrriage
Anisotropy	0.596	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5578	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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

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	0.71	0/5336	0.88	3/7228 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ASN	CB-CA-C	5.76	121.92	110.40
1	A	380	THR	CB-CA-C	5.64	126.84	111.60
1	A	380	THR	N-CA-CB	-5.38	100.08	110.30

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	5202	0	5066	73	0
2	A	53	0	31	1	0
3	A	30	0	18	1	0
4	A	293	0	0	10	0
All	All	5578	0	5115	74	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 (74) 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:496:GLN:HG2	4:A:936:HOH:O	1.84	0.76
1:A:349:ARG:HD2	1:A:425:ASP:OD2	1.91	0.70
1:A:237:ILE:HG23	1:A:297:LEU:HD11	1.76	0.68
1:A:608:SER:HB2	4:A:976:HOH:O	1.93	0.67
1:A:496:GLN:HB3	1:A:595:ILE:HD11	1.76	0.67
1:A:254:LEU:HD13	1:A:372:PHE:CE1	2.29	0.67
1:A:122:LYS:HE3	4:A:803:HOH:O	1.97	0.64
1:A:485:GLN:HE21	1:A:485:GLN:HA	1.62	0.64
1:A:253:GLY:HA2	1:A:424:HIS:O	2.00	0.61
1:A:118:THR:CG2	4:A:1024:HOH:O	2.48	0.60
1:A:596:ARG:HG3	1:A:597:LEU:N	2.15	0.60
1:A:560:GLU:HB2	4:A:837:HOH:O	2.02	0.58
1:A:218:SER:N	1:A:219:PRO:CD	2.66	0.58
1:A:132:ARG:NH1	1:A:329:GLU:OE1	2.35	0.58
1:A:60:TYR:OH	1:A:380:THR:CG2	2.52	0.58
1:A:124:VAL:O	1:A:363:ILE:HA	2.04	0.57
1:A:237:ILE:HG23	1:A:297:LEU:CD1	2.35	0.57
1:A:222:PRO:HA	1:A:231:TYR:CZ	2.40	0.57
1:A:446:GLN:NE2	1:A:448:ASN:HD21	2.03	0.57
1:A:118:THR:HG22	4:A:1024:HOH:O	2.07	0.55
1:A:491:HIS:O	1:A:496:GLN:NE2	2.42	0.53
1:A:173:ILE:HB	1:A:295:VAL:HG22	1.90	0.52
1:A:192:LYS:HG3	1:A:193:PRO:HD2	1.91	0.52
1:A:553:ASP:OD2	1:A:555:THR:OG1	2.22	0.51
1:A:128:THR:OG1	1:A:368:TYR:OH	2.27	0.50
1:A:189:VAL:HG11	1:A:496:GLN:HG3	1.93	0.50
1:A:485:GLN:HG3	4:A:1011:HOH:O	2.11	0.50
1:A:71:ASP:OD2	1:A:491:HIS:HE1	1.95	0.49
1:A:365:PHE:HB3	1:A:368:TYR:HD2	1.76	0.49
1:A:349:ARG:NH2	1:A:419:ALA:O	2.45	0.49
1:A:172:LYS:HD2	1:A:561:TRP:NE1	2.28	0.49
1:A:289:TRP:HB3	1:A:295:VAL:HG23	1.95	0.48
1:A:645:LYS:HE3	1:A:645:LYS:HA	1.95	0.48
1:A:353:MET:CE	1:A:436:ASP:HB3	2.43	0.48
1:A:446:GLN:HE21	1:A:448:ASN:HD21	1.60	0.48
1:A:218:SER:N	1:A:219:PRO:HD2	2.30	0.47
1:A:318:ARG:NH2	1:A:558:ASP:OD2	2.40	0.47
1:A:457:LEU:HD12	1:A:498:PHE:CD2	2.50	0.46
1:A:609:LEU:HD22	1:A:635:ILE:HD11	1.97	0.46
1:A:576:ALA:N	1:A:577:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:TYR:OH	1:A:380:THR:HG23	2.15	0.46
1:A:200:GLU:O	1:A:201:SER:C	2.54	0.46
1:A:499:VAL:HG21	1:A:594:GLY:C	2.36	0.46
1:A:40:ARG:HG3	4:A:1028:HOH:O	2.17	0.45
1:A:71:ASP:OD2	1:A:491:HIS:CE1	2.69	0.44
1:A:633:GLN:CA	1:A:633:GLN:HE21	2.29	0.44
1:A:118:THR:HG21	4:A:1054:HOH:O	2.17	0.43
1:A:566:LYS:HD3	1:A:566:LYS:N	2.33	0.43
1:A:309:LYS:NZ	1:A:321:HIS:O	2.50	0.43
2:A:701:FAD:C10	3:A:703:TRP:HA	2.48	0.43
1:A:446:GLN:HB3	1:A:448:ASN:OD1	2.17	0.43
1:A:645:LYS:HA	1:A:645:LYS:CE	2.48	0.43
1:A:357:PRO:CG	1:A:360:LEU:HD12	2.49	0.43
1:A:202:PRO:HG2	1:A:431:GLY:HA3	2.01	0.43
1:A:224:THR:HA	1:A:514:GLU:OE1	2.18	0.42
1:A:348:TYR:O	1:A:351:THR:HB	2.19	0.42
1:A:597:LEU:HD22	1:A:597:LEU:C	2.39	0.42
1:A:19:GLU:HB3	1:A:388:HIS:CD2	2.54	0.42
1:A:65:VAL:HG22	1:A:479:GLY:C	2.39	0.42
1:A:483:LEU:O	1:A:487:VAL:HG23	2.19	0.42
1:A:487:VAL:O	1:A:491:HIS:HD2	2.03	0.42
1:A:313:TYR:O	1:A:314:ALA:HB3	2.19	0.42
1:A:4:VAL:O	1:A:27:PHE:HA	2.19	0.42
1:A:103:GLU:HB2	1:A:110:LEU:HB3	2.01	0.42
1:A:331:PRO:HG2	1:A:346:TYR:CE2	2.55	0.42
1:A:262:ILE:HD12	1:A:283:LEU:HD21	2.02	0.41
1:A:201:SER:N	1:A:202:PRO:HD3	2.35	0.41
1:A:506:ASN:HB2	4:A:972:HOH:O	2.21	0.41
1:A:353:MET:HE2	1:A:436:ASP:HB3	2.03	0.41
1:A:224:THR:HG22	1:A:231:TYR:OH	2.20	0.41
1:A:593:LYS:O	1:A:596:ARG:HG2	2.21	0.41
1:A:304:ILE:HD12	1:A:310:THR:O	2.22	0.40
1:A:305:ASN:HD22	1:A:305:ASN:HA	1.59	0.40
1:A:370:ARG:O	1:A:427:THR:HA	2.21	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	623/679 (92%)	589 (94%)	31 (5%)	3 (0%)	29 31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	ASN
1	A	10	GLY
1	A	532	GLY

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	571/603 (95%)	519 (91%)	52 (9%)	9 9

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	33	GLU
1	A	37	VAL
1	A	40	ARG
1	A	65	VAL
1	A	93	LYS
1	A	118	THR
1	A	145	VAL

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Mol	Chain	Res	Type
1	A	177	THR
1	A	184	ASP
1	A	186	GLU
1	A	190	LEU
1	A	192	LYS
1	A	215	LEU
1	A	231	TYR
1	A	236	LEU
1	A	254	LEU
1	A	271	ASP
1	A	275	ASN
1	A	305	ASN
1	A	308	LYS
1	A	310	THR
1	A	319	SER
1	A	330	GLN
1	A	341	GLU
1	A	347	LEU
1	A	351	THR
1	A	359	ARG
1	A	366	LEU
1	A	380	THR
1	A	402	GLN
1	A	423	LYS
1	A	426	HIS
1	A	456	LEU
1	A	457	LEU
1	A	472	LYS
1	A	483	LEU
1	A	485	GLN
1	A	490	LYS
1	A	496	GLN
1	A	509	SER
1	A	546	GLN
1	A	552	VAL
1	A	566	LYS
1	A	596	ARG
1	A	597	LEU
1	A	604	SER
1	A	607	SER
1	A	633	GLN
1	A	635	ILE

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Mol	Chain	Res	Type
1	A	640	ARG
1	A	645	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	83	HIS
1	A	144	HIS
1	A	169	ASN
1	A	188	GLN
1	A	264	GLN
1	A	305	ASN
1	A	401	HIS
1	A	426	HIS
1	A	446	GLN
1	A	485	GLN
1	A	491	HIS
1	A	500	GLN
1	A	592	ASN
1	A	633	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](#)

3 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
3	TRP	A	703	-	14,16,16	0.63	0	16,22,22	1.22	2 (12%)
2	FAD	A	701	-	53,58,58	0.73	0	68,89,89	0.95	3 (4%)
3	TRP	A	702	-	14,16,16	0.91	1 (7%)	16,22,22	1.22	2 (12%)

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	TRP	A	703	-	-	1/7/8/8	0/2/2/2
2	FAD	A	701	-	-	2/30/50/50	0/6/6/6
3	TRP	A	702	-	-	1/7/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	TRP	OXT-C	-2.07	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	TRP	OXT-C-CA	3.14	124.08	113.38
3	A	702	TRP	OXT-C-CA	2.66	122.44	113.38
3	A	702	TRP	CH2-CZ2-CE2	-2.48	116.51	120.08
3	A	703	TRP	O-C-CA	-2.39	113.69	122.14
2	A	701	FAD	C4-N3-C2	-2.23	121.53	125.64
2	A	701	FAD	C5A-C6A-N6A	2.09	123.53	120.35
2	A	701	FAD	O5'-P-O1P	-2.01	101.21	109.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

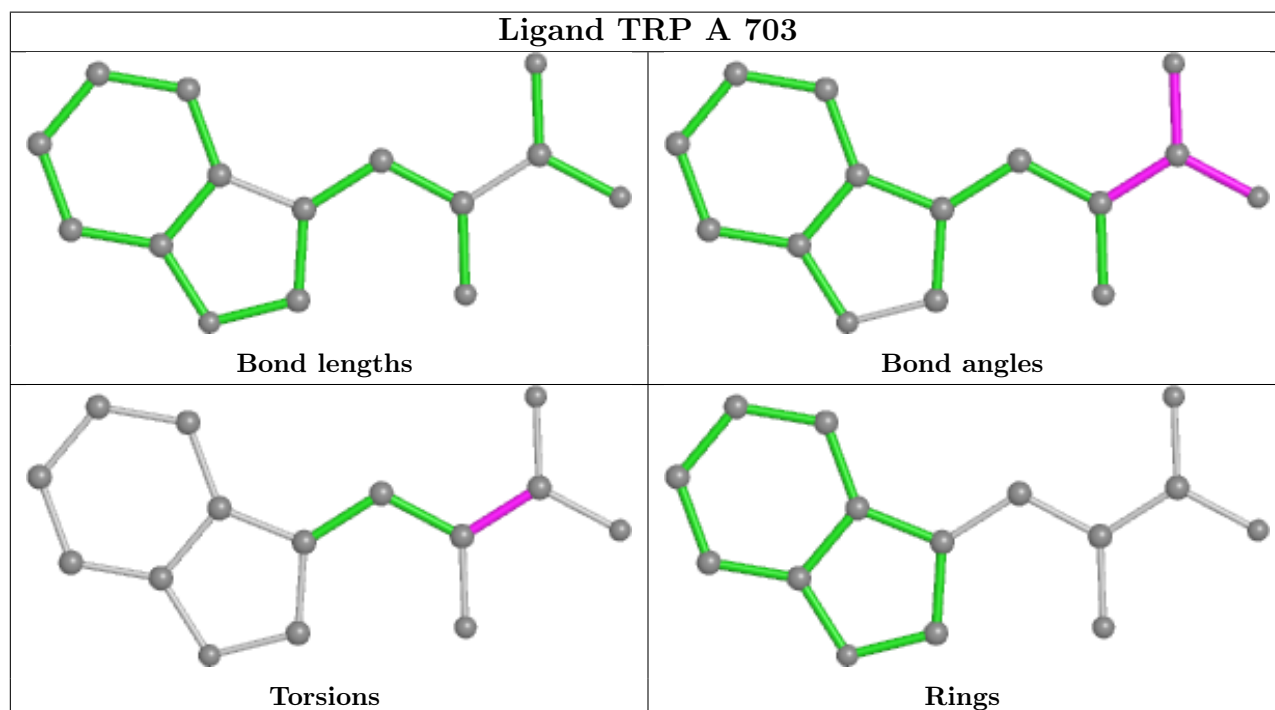
Mol	Chain	Res	Type	Atoms
2	A	701	FAD	N10-C1'-C2'-C3'
3	A	702	TRP	CA-CB-CG-CD1
2	A	701	FAD	O4B-C4B-C5B-O5B
3	A	703	TRP	OXT-C-CA-CB

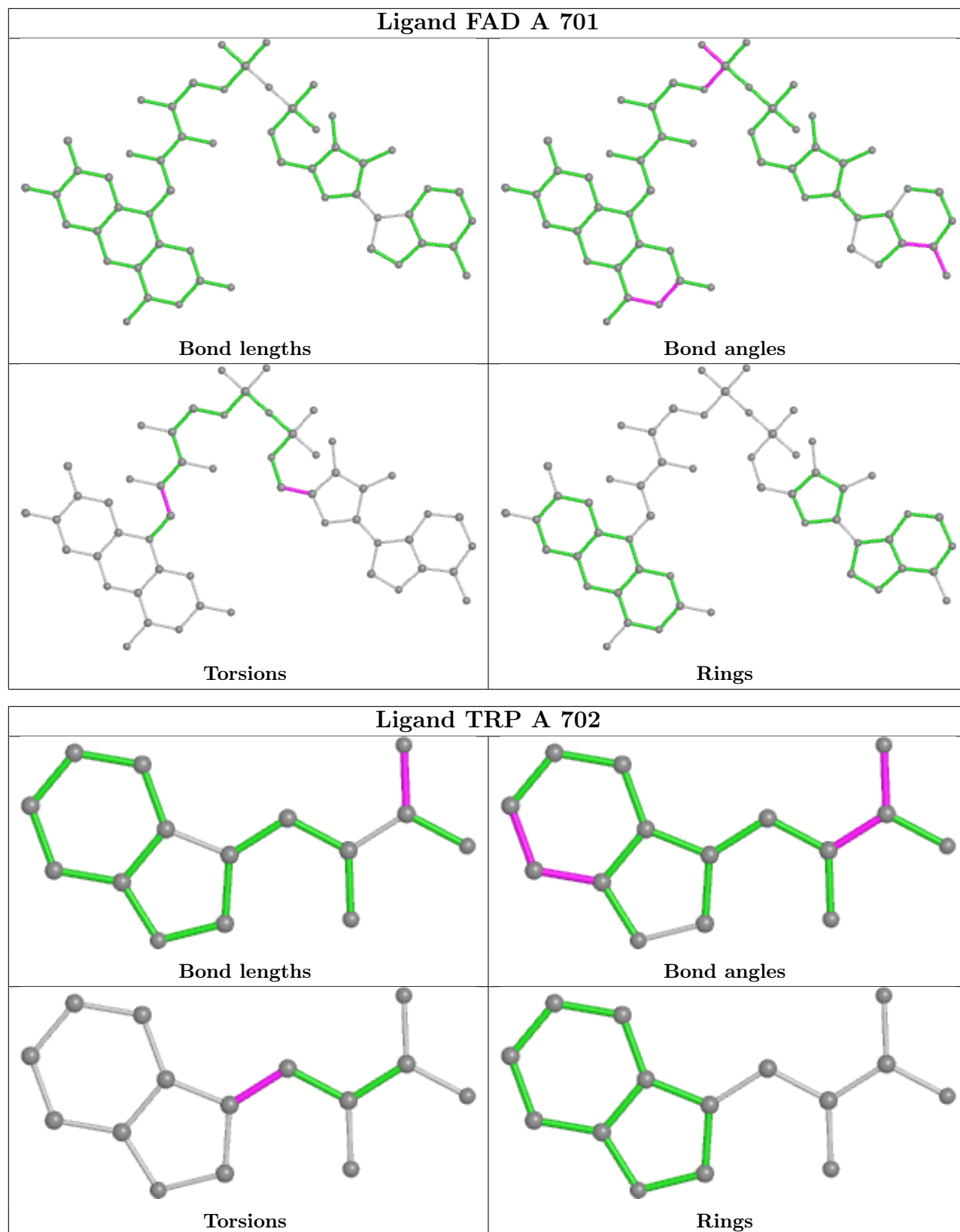
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	TRP	1	0
2	A	701	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 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	629/679 (92%)	-0.12	14 (2%) 62 59	21, 39, 69, 94	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	578	ASN	5.2
1	A	612	SER	4.6
1	A	577	PRO	4.0
1	A	555	THR	3.9
1	A	143	ASN	3.2
1	A	607	SER	3.1
1	A	317	GLU	2.4
1	A	418	ALA	2.4
1	A	379	ILE	2.3
1	A	547	VAL	2.3
1	A	199	LEU	2.2
1	A	196	LEU	2.2
1	A	553	ASP	2.2
1	A	141	PHE	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](#)

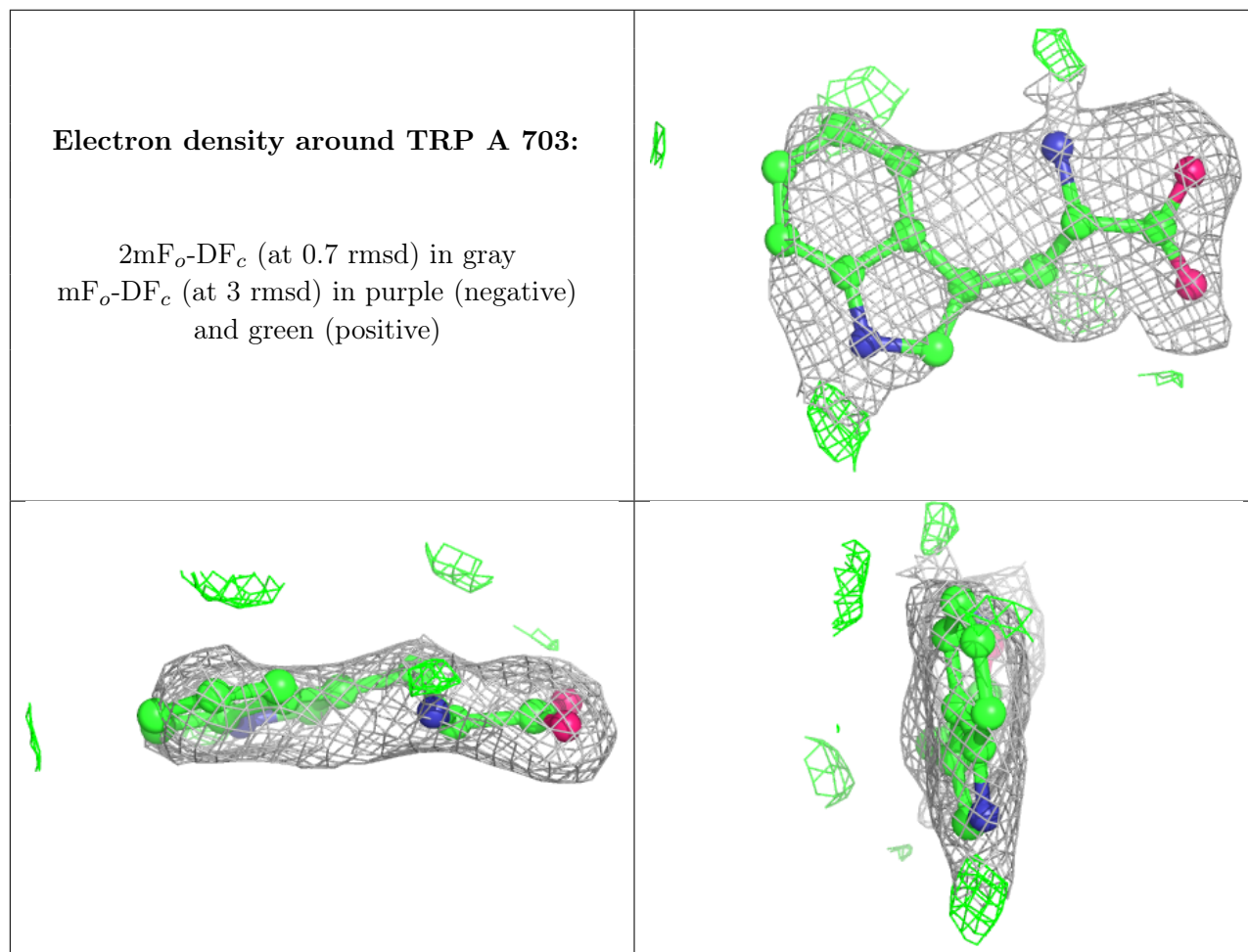
There are no monosaccharides in this entry.

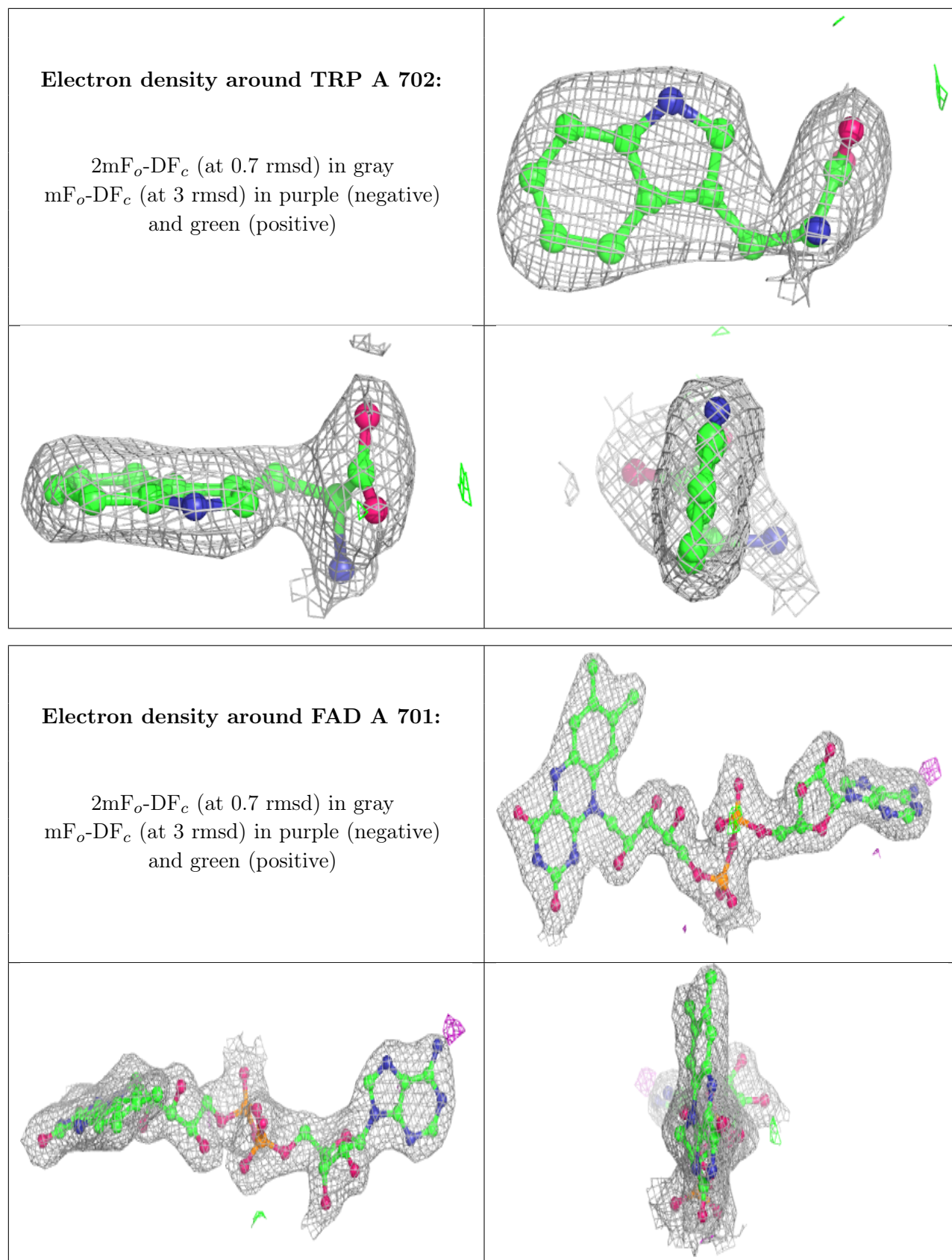
6.4 Ligands [i](#)

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, 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	TRP	A	703	15/15	0.73	0.38	53,74,78,79	0
3	TRP	A	702	15/15	0.92	0.20	30,33,36,37	0
2	FAD	A	701	53/53	0.96	0.11	23,27,33,35	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.