



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:54 AM UTC

PDB ID : 8D3H / pdb_00008d3h
Title : Crystal structure of human Apoptosis-Inducing Factor (AIF) W196A mutant complexed with 7-chloroquinolin-4-amine
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Deposited on : 2022-06-01
Resolution : 2.51 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)
Xtriage (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

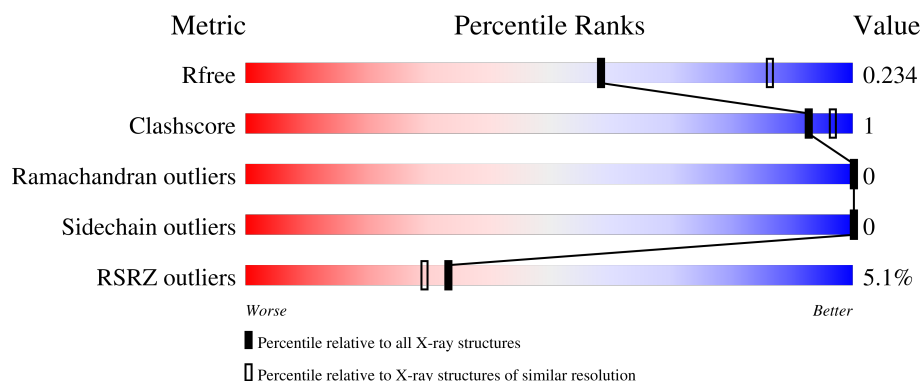
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	543	
2	B	543	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13245 atoms, of which 6443 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 Apoptosis-inducing factor 1, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	432	6430	2068	3190	566	595	11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	initiating methionine	UNP O95831
A	196	ALA	TRP	engineered mutation	UNP O95831
A	614	LEU	-	expression tag	UNP O95831
A	615	GLU	-	expression tag	UNP O95831
A	616	VAL	-	expression tag	UNP O95831
A	617	LEU	-	expression tag	UNP O95831
A	618	PHE	-	expression tag	UNP O95831
A	619	GLN	-	expression tag	UNP O95831

- Molecule 2 is a protein called Apoptosis-inducing factor 1, mitochondrial.

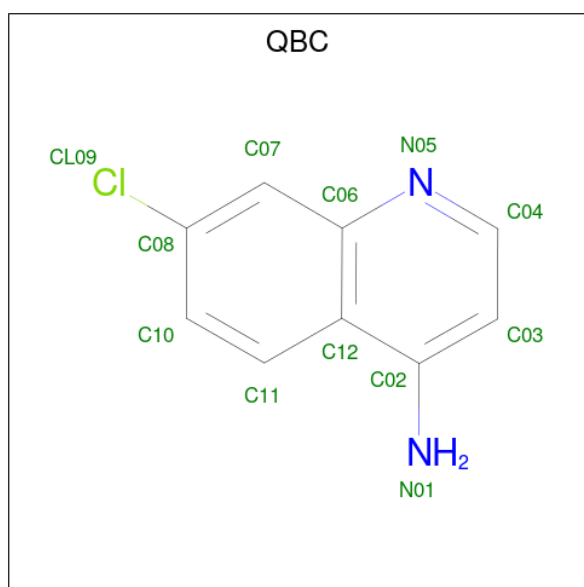
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	434	6421	2067	3173	573	597	11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	77	MET	-	initiating methionine	UNP O95831
B	196	ALA	TRP	engineered mutation	UNP O95831
B	614	LEU	-	expression tag	UNP O95831
B	615	GLU	-	expression tag	UNP O95831
B	616	VAL	-	expression tag	UNP O95831
B	617	LEU	-	expression tag	UNP O95831
B	618	PHE	-	expression tag	UNP O95831
B	619	GLN	-	expression tag	UNP O95831

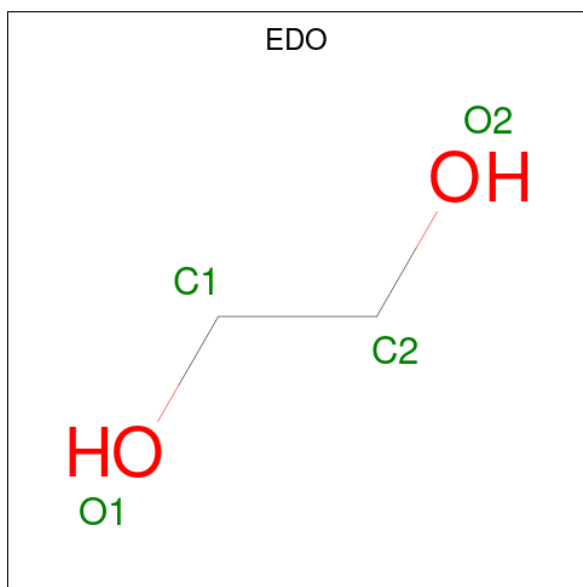
- # FAD

- Molecule 4 is 7-chloroquinolin-4-amine (CCD ID: QBC) (formula: $\text{C}_9\text{H}_7\text{ClN}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	H	N	0	0
			19	9	1	7	2		
4	B	1	Total	C	Cl	H	N	0	0
			19	9	1	7	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

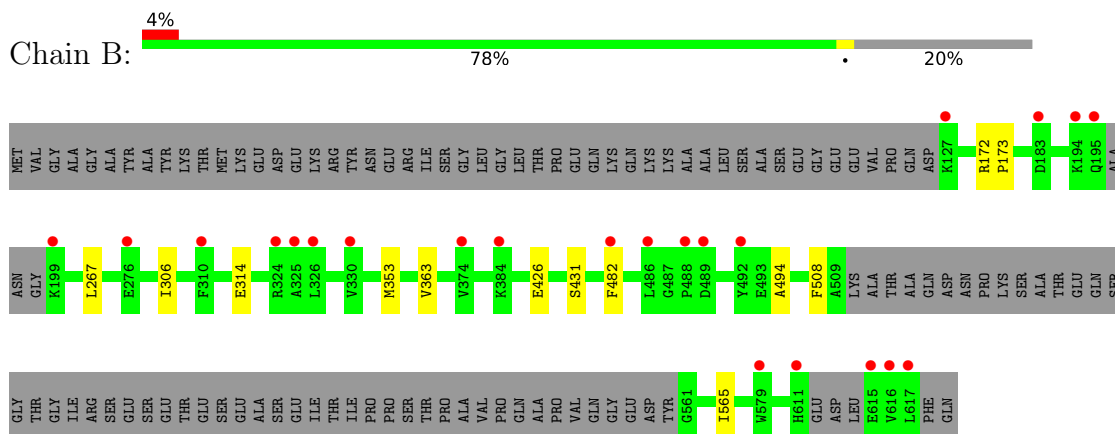
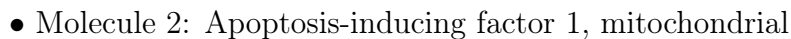


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	84	Total O 84 84	0	0
6	B	96	Total O 96 96	0	0

- Molecule 1: Apoptosis-inducing factor 1, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.79Å 114.77Å 120.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.36 – 2.51 29.36 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.36-2.51) 99.5 (29.36-2.51)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.204 , 0.231 0.207 , 0.234	Depositor DCC
R_{free} test set	2145 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13245	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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, CSX, EDO, QBC

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	0.10	0/3298	0.24	0/4471
2	B	0.10	0/3296	0.25	0/4466
All	All	0.10	0/6594	0.25	0/8937

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	3240	3190	3195	12	0
2	B	3248	3173	3180	9	0
3	A	53	30	31	0	0
3	B	53	30	31	0	0
4	A	12	7	0	0	0
4	B	12	7	0	1	0
5	A	4	6	6	0	0
6	A	84	0	0	1	0
6	B	96	0	0	0	0
All	All	6802	6443	6443	19	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 1.

All (19) 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)
2:B:267:LEU:HD11	2:B:306:ILE:HG21	1.72	0.71
1:A:267:LEU:HD11	1:A:306:ILE:HG21	1.76	0.68
1:A:508:PHE:CZ	1:A:565:ILE:HD11	2.36	0.60
1:A:265:ARG:NH1	1:A:401:GLU:OE1	2.36	0.59
1:A:426:GLU:OE1	2:B:431:SER:OG	2.23	0.55
2:B:508:PHE:CZ	2:B:565:ILE:HD11	2.43	0.54
2:B:172:ARG:N	2:B:173:PRO:CD	2.76	0.49
1:A:172:ARG:N	1:A:173:PRO:CD	2.76	0.49
2:B:482:PHE:CE2	2:B:494:ALA:HB3	2.49	0.48
1:A:508:PHE:HZ	1:A:565:ILE:HD11	1.77	0.47
1:A:280:ARG:NH1	1:A:377:GLY:O	2.43	0.47
1:A:584:ARG:NH2	6:A:805:HOH:O	2.48	0.46
2:B:508:PHE:HZ	2:B:565:ILE:HD11	1.79	0.45
1:A:431:SER:OG	2:B:426:GLU:OE1	2.31	0.45
1:A:301:LYS:HD3	1:A:328:THR:HG22	1.97	0.45
2:B:314:GLU:OE2	4:B:702:QBC:N01	2.49	0.45
1:A:158:ARG:NH2	1:A:220:ILE:O	2.52	0.43
1:A:564:VAL:HG23	1:A:578:LEU:HD23	1.99	0.43
2:B:353:MET:HG3	2:B:363:VAL:HG11	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	427/543 (79%)	412 (96%)	15 (4%)	0	100	100
2	B	424/543 (78%)	410 (97%)	14 (3%)	0	100	100
All	All	851/1086 (78%)	822 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	327/443 (74%)	327 (100%)	0	100	100
2	B	325/442 (74%)	325 (100%)	0	100	100
All	All	652/885 (74%)	652 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	457	HIS
1	A	602	ASN
2	B	457	HIS
2	B	602	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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	CSX	B	256	2	3,6,7	0.99	0	1,6,8	0.50	0
2	CSX	B	441	2	3,6,7	0.96	0	1,6,8	1.07	0
1	CSX	A	441	1	3,6,7	0.98	0	1,6,8	1.57	0

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	CSX	B	256	2	-	0/2/5/7	-
2	CSX	B	441	2	-	0/2/5/7	-
1	CSX	A	441	1	-	1/2/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	441	CSX	C-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
4	QBC	A	702	-	13,13,13	1.75	4 (30%)	18,18,18	1.30	3 (16%)
5	EDO	A	703	-	3,3,3	0.45	0	2,2,2	0.38	0
3	FAD	B	701	-	58,58,58	1.45	4 (6%)	85,89,89	0.94	3 (3%)
3	FAD	A	701	-	58,58,58	1.46	4 (6%)	85,89,89	0.92	3 (3%)
4	QBC	B	702	-	13,13,13	1.75	5 (38%)	18,18,18	1.31	3 (16%)

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
4	QBC	A	702	-	-	-	0/2/2/2
5	EDO	A	703	-	-	0/1/1/1	-
3	FAD	B	701	-	-	5/34/50/50	0/6/6/6
3	FAD	A	701	-	-	5/34/50/50	0/6/6/6
4	QBC	B	702	-	-	-	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	FAD	C9-C9A	6.25	1.49	1.39
3	B	701	FAD	C9-C9A	6.19	1.49	1.39
3	B	701	FAD	C6-C5X	6.12	1.49	1.40
3	A	701	FAD	C6-C5X	6.04	1.49	1.40
3	B	701	FAD	O5'-C5'	3.26	1.56	1.44
3	A	701	FAD	O5'-C5'	3.25	1.56	1.44
4	B	702	QBC	C07-C06	-2.80	1.37	1.41
4	A	702	QBC	C07-C06	-2.78	1.37	1.41
4	B	702	QBC	C12-C06	-2.64	1.38	1.42
4	A	702	QBC	C12-C06	-2.63	1.38	1.42
4	B	702	QBC	C02-C12	-2.60	1.36	1.43
4	A	702	QBC	C02-C12	-2.59	1.36	1.43
4	A	702	QBC	C06-N05	-2.19	1.33	1.37
4	B	702	QBC	C06-N05	-2.14	1.33	1.37
3	B	701	FAD	C1'-C2'	2.12	1.55	1.52
3	A	701	FAD	C1'-C2'	2.09	1.55	1.52
4	B	702	QBC	C08-CL09	2.00	1.79	1.74

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	702	QBC	C03-C04-N05	-3.31	119.69	124.60
4	A	702	QBC	C03-C04-N05	-3.27	119.74	124.60
3	A	701	FAD	C4-N3-C2	-2.60	121.02	125.64
3	B	701	FAD	C4-N3-C2	-2.59	121.04	125.64
3	B	701	FAD	C4'-C3'-C2'	-2.51	109.40	113.57
3	B	701	FAD	C5'-C4'-C3'	-2.42	107.66	112.22
4	B	702	QBC	C07-C06-N05	-2.29	115.38	118.01
4	A	702	QBC	C07-C06-N05	-2.21	115.47	118.01
4	B	702	QBC	C07-C06-C12	2.19	122.02	119.58
4	A	702	QBC	C07-C06-C12	2.16	121.99	119.58
3	A	701	FAD	C5'-C4'-C3'	-2.10	108.25	112.22
3	A	701	FAD	C4'-C3'-C2'	-2.01	110.22	113.57

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	FAD	C3B-C4B-C5B-O5B
3	B	701	FAD	C3B-C4B-C5B-O5B
3	A	701	FAD	PA-O3P-P-O5'
3	B	701	FAD	PA-O3P-P-O5'
3	A	701	FAD	O4B-C4B-C5B-O5B
3	B	701	FAD	O4B-C4B-C5B-O5B
3	B	701	FAD	C2B-C1B-N9A-C8A
3	A	701	FAD	C2B-C1B-N9A-C8A
3	A	701	FAD	P-O3P-PA-O2A
3	B	701	FAD	P-O3P-PA-O2A

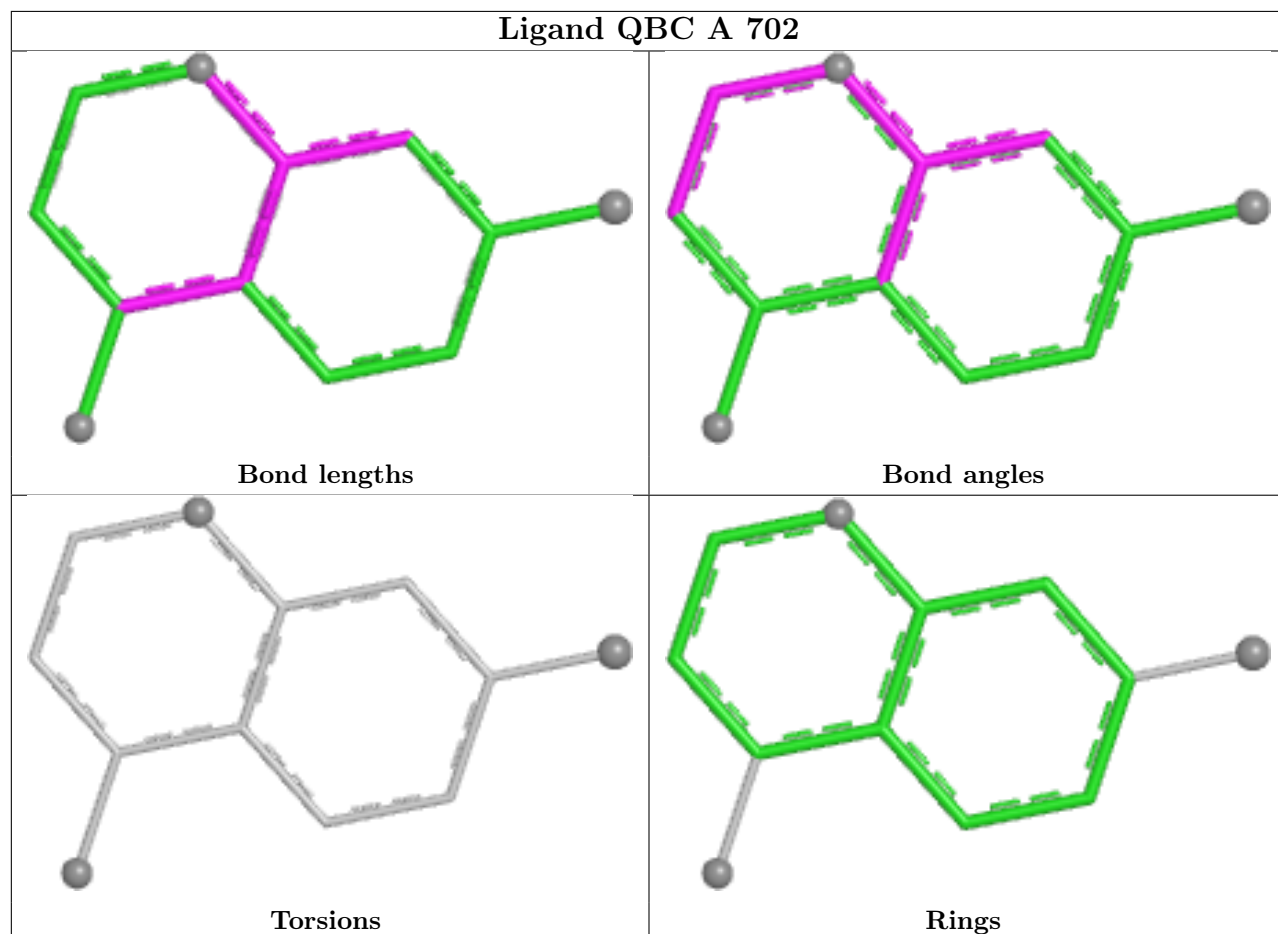
There are no ring outliers.

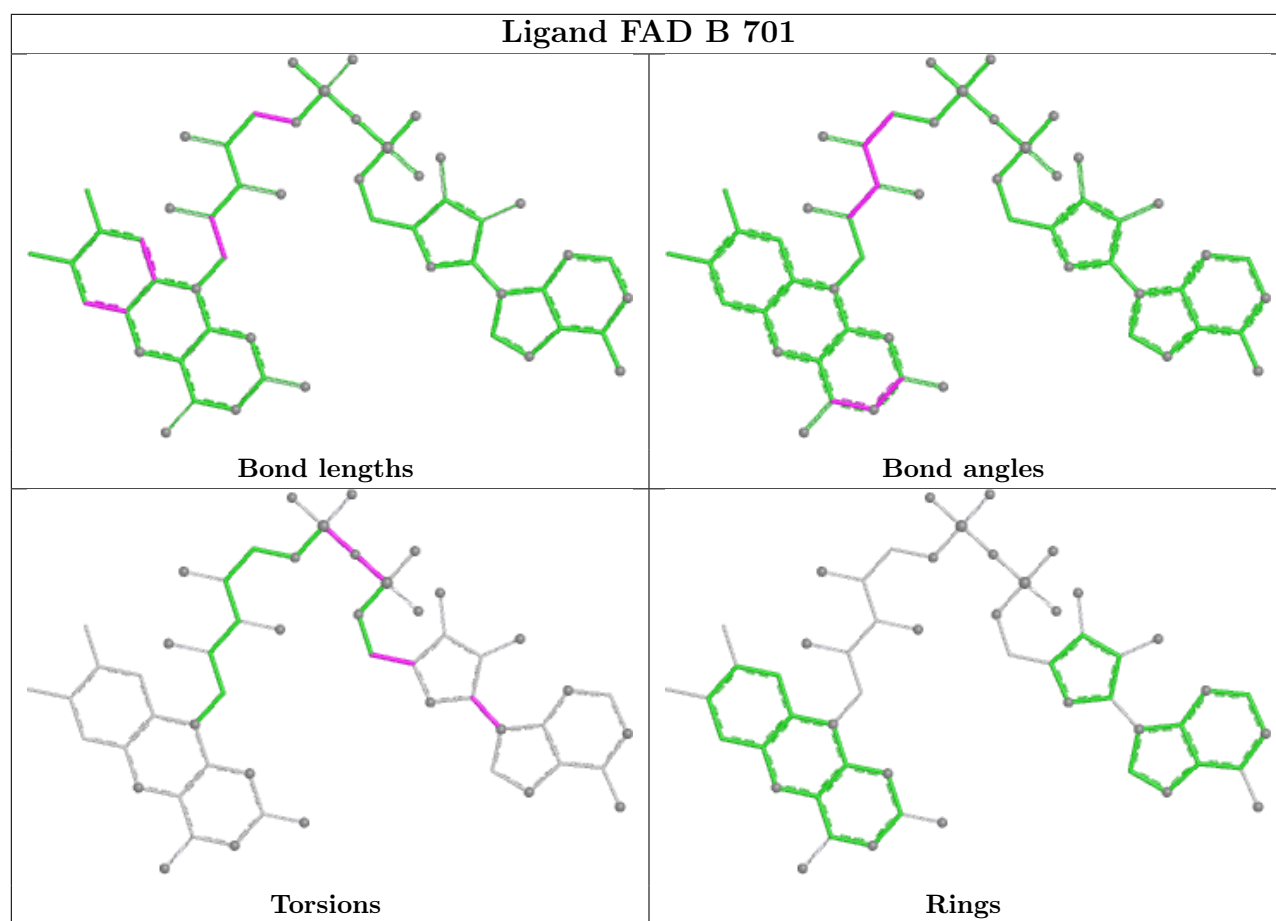
1 monomer is involved in 1 short contact:

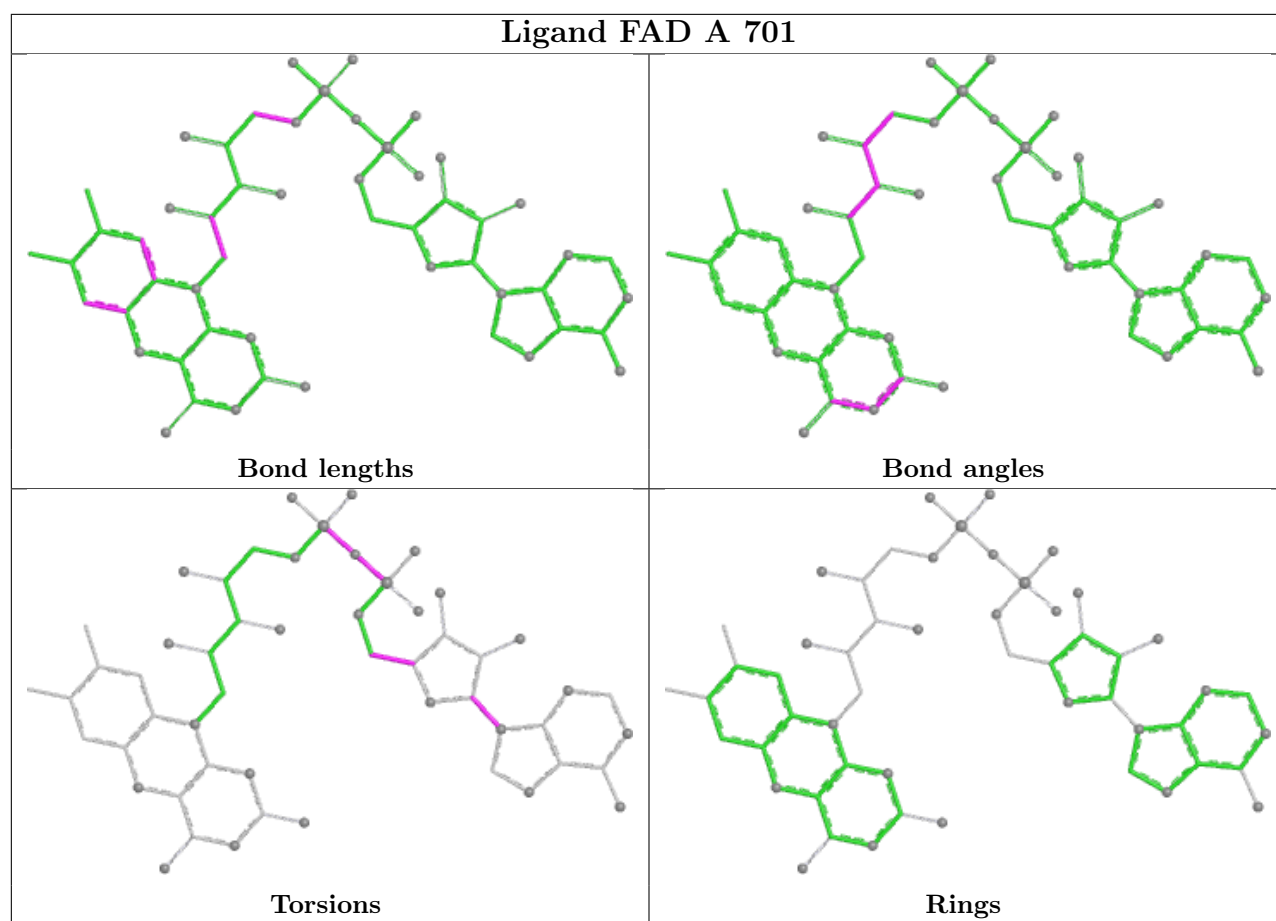
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	702	QBC	1	0

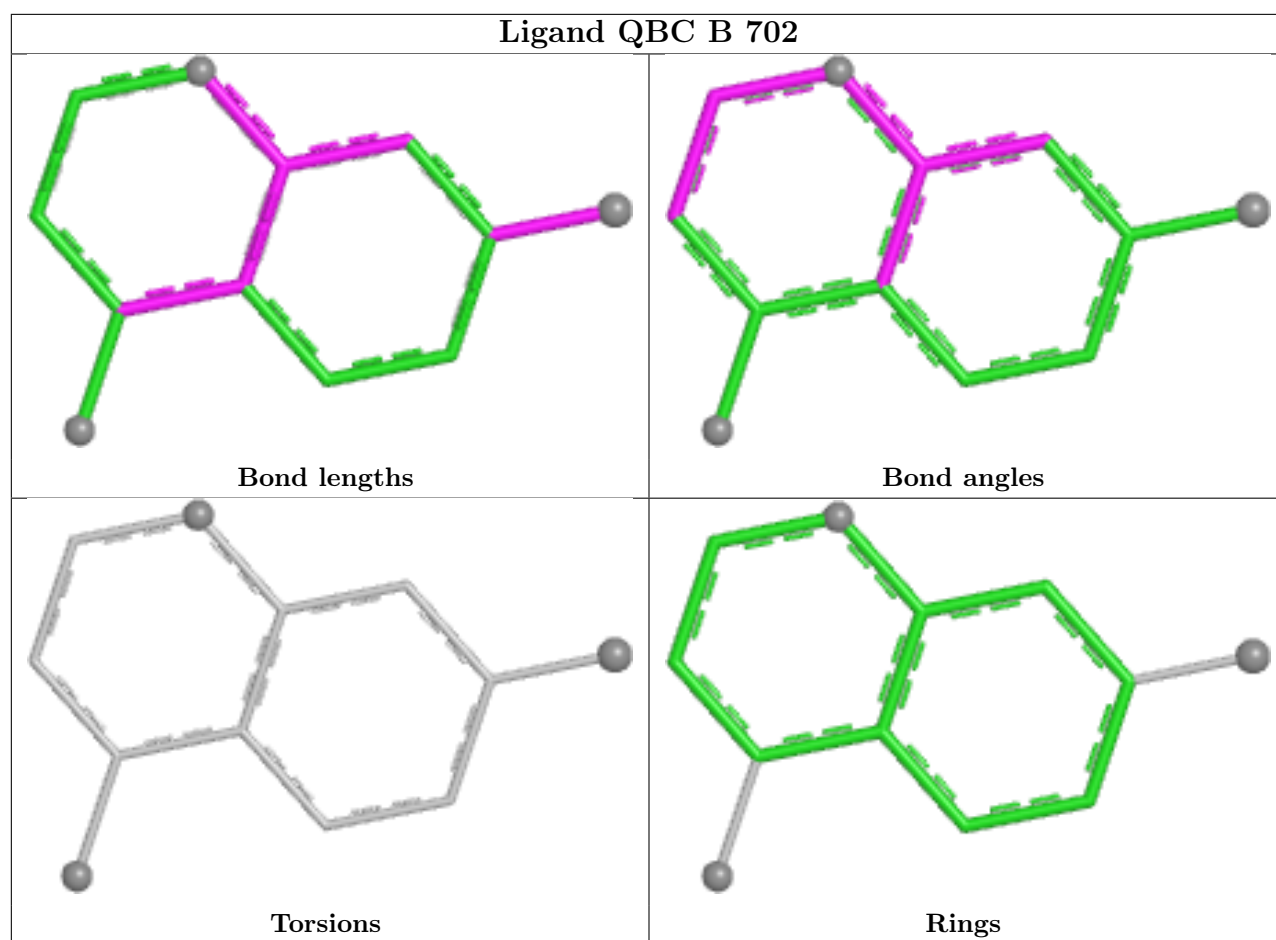
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains

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	431/543 (79%)	0.47	21 (4%) 35 31	44, 70, 99, 129	0
2	B	432/543 (79%)	0.35	23 (5%) 32 28	42, 64, 101, 127	0
All	All	863/1086 (79%)	0.41	44 (5%) 33 29	42, 67, 100, 129	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	276	GLU	5.7
1	A	197	ASN	4.9
1	A	509	ALA	4.8
1	A	489	ASP	4.7
2	B	489	ASP	4.2
1	A	492	TYR	4.0
2	B	324	ARG	3.9
2	B	127	LYS	3.7
2	B	374	VAL	3.6
1	A	326	LEU	3.5
2	B	492	TYR	3.4
2	B	488	PRO	3.4
1	A	561	GLY	3.4
1	A	482	PHE	3.3
2	B	199	LYS	3.2
1	A	376	SER	3.1
1	A	570	ASP	3.1
2	B	616	VAL	3.1
2	B	326	LEU	3.0
1	A	199	LYS	3.0
2	B	617	LEU	3.0
2	B	482	PHE	2.9
1	A	488	PRO	2.7
2	B	615	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	330	VAL	2.7
2	B	325	ALA	2.6
2	B	194	LYS	2.6
1	A	486	LEU	2.5
1	A	562	LYS	2.5
2	B	579	TRP	2.4
2	B	183	ASP	2.4
1	A	196	ALA	2.3
2	B	486	LEU	2.3
1	A	194	LYS	2.3
1	A	579	TRP	2.2
2	B	384	LYS	2.2
1	A	611	HIS	2.1
1	A	310	PHE	2.1
1	A	487	GLY	2.1
1	A	563	GLY	2.1
1	A	355	LYS	2.1
2	B	310	PHE	2.1
2	B	195	GLN	2.0
2	B	611	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSX	A	441	7/8	0.90	0.12	41,44,49,51	0
2	CSX	B	256	7/8	0.91	0.13	40,41,52,54	0
2	CSX	B	441	7/8	0.95	0.09	39,40,50,56	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

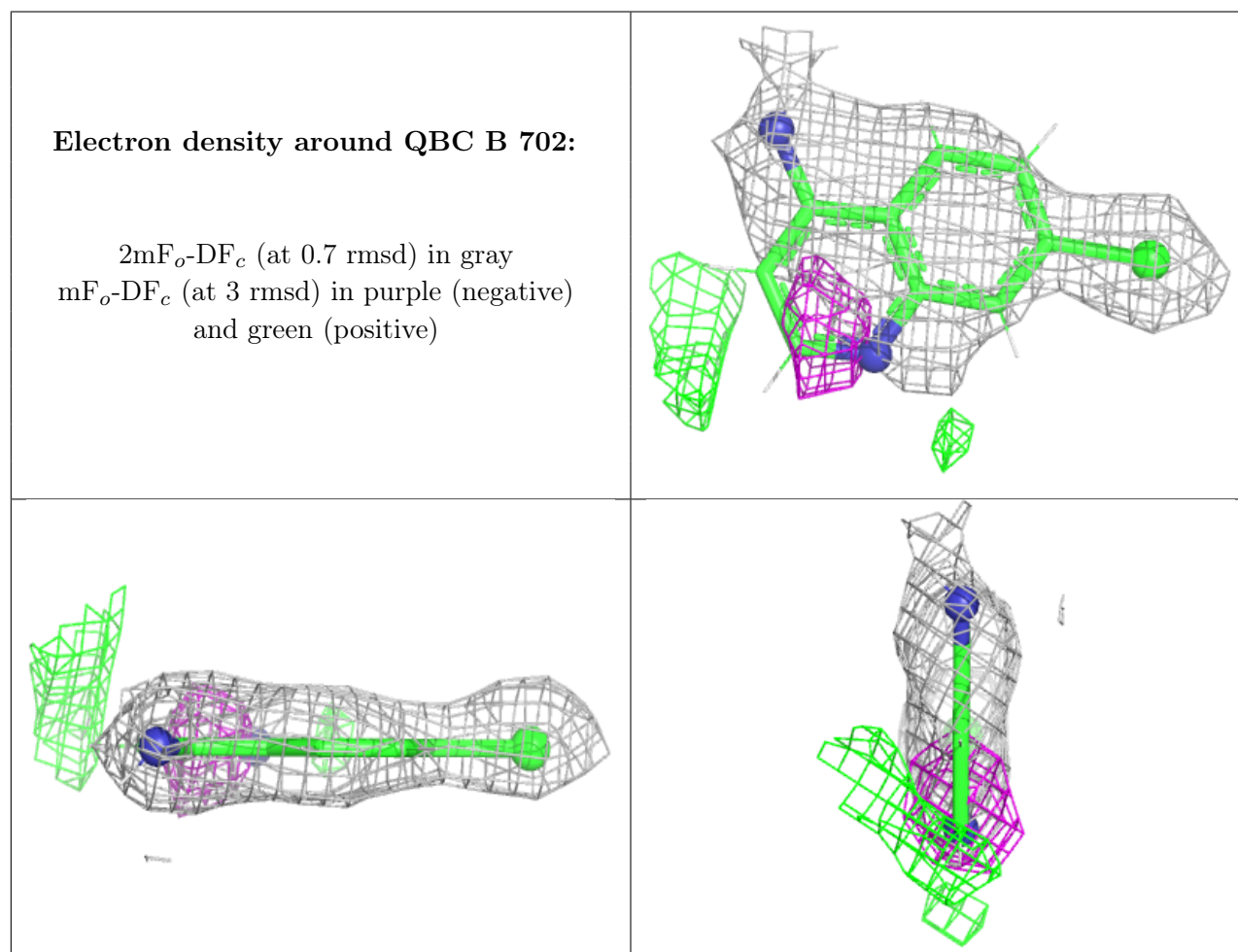
6.4 Ligands [i](#)

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.

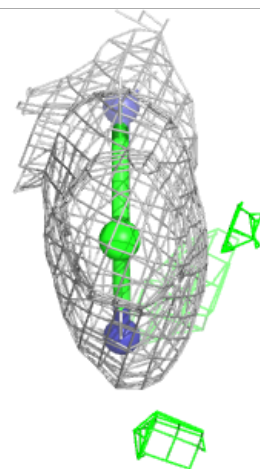
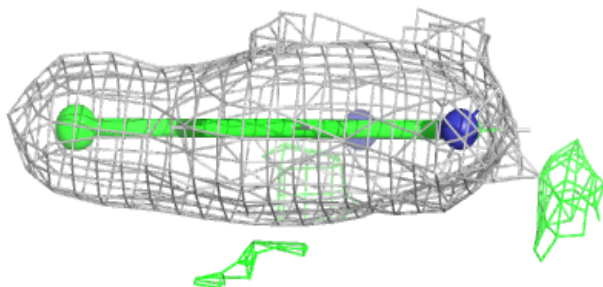
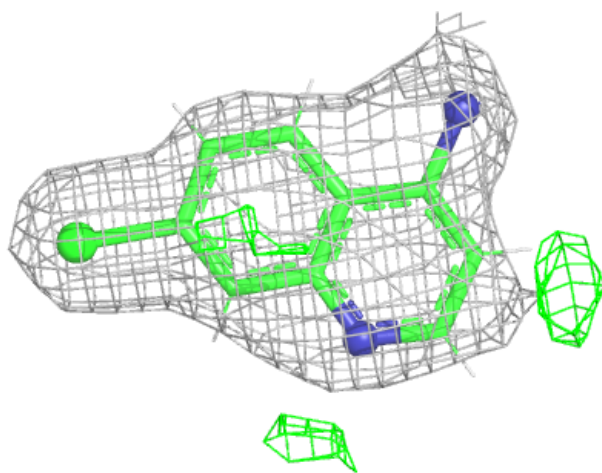
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	QBC	B	702	12/12	0.85	0.19	48,51,61,61	19
5	EDO	A	703	4/4	0.86	0.22	43,52,55,60	0
4	QBC	A	702	12/12	0.90	0.14	48,54,65,66	19
3	FAD	A	701	53/53	0.92	0.13	50,61,75,240	0
3	FAD	B	701	53/53	0.94	0.10	48,55,70,132	0

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.



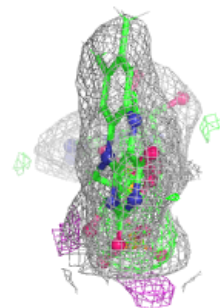
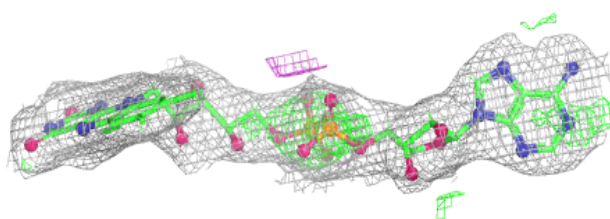
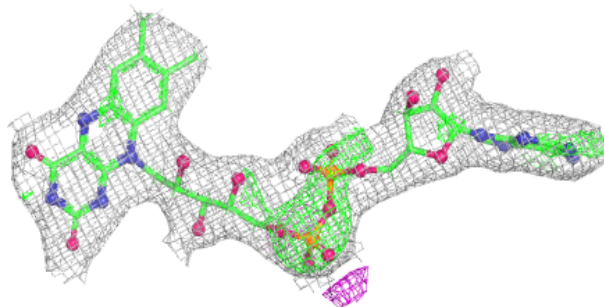
Electron density around QBC A 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

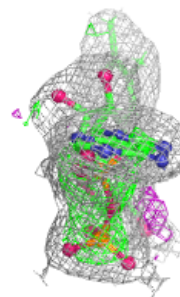
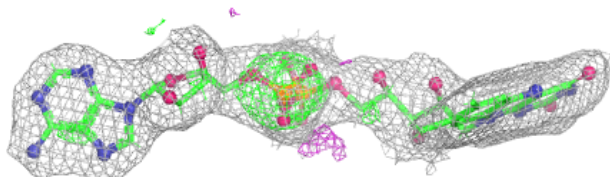
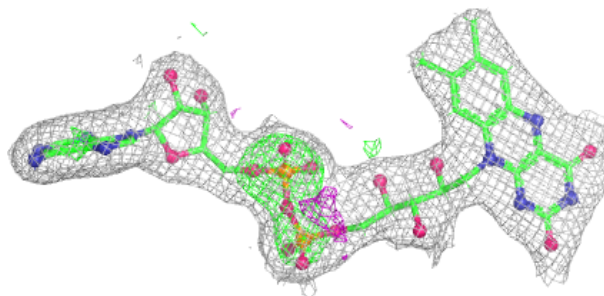


Electron density around FAD A 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD B 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.