



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2024 – 01:22 PM EDT

PDB ID : 4K03
Title : Crystal structure of Drosophila Cryochrome
Authors : Berndt, A.; Wolf, E.
Deposited on : 2013-04-03
Resolution : 3.20 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 ⓘ 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

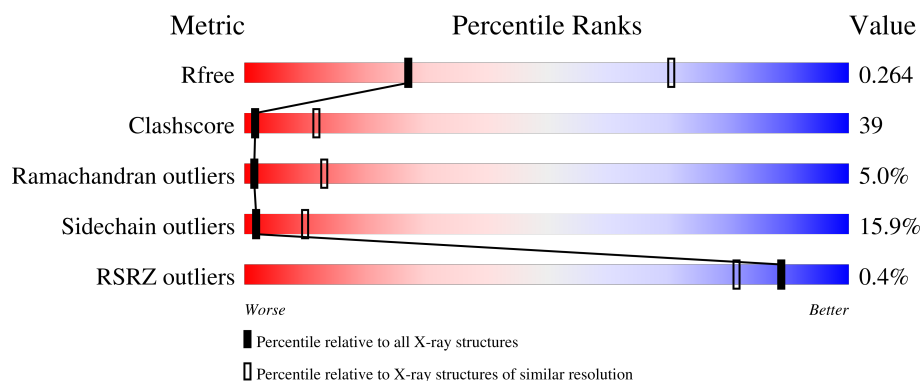
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

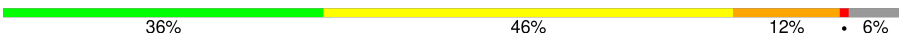

The reported resolution of this entry is 3.20 Å.

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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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	561	
1	B	561	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8746 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 Cryptochrome-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4238	2707	749	758	24			
1	B	543	Total	C	N	O	S	0	0	0
			4350	2775	769	781	25			

There are 38 discrepancies between the modelled and reference sequences:

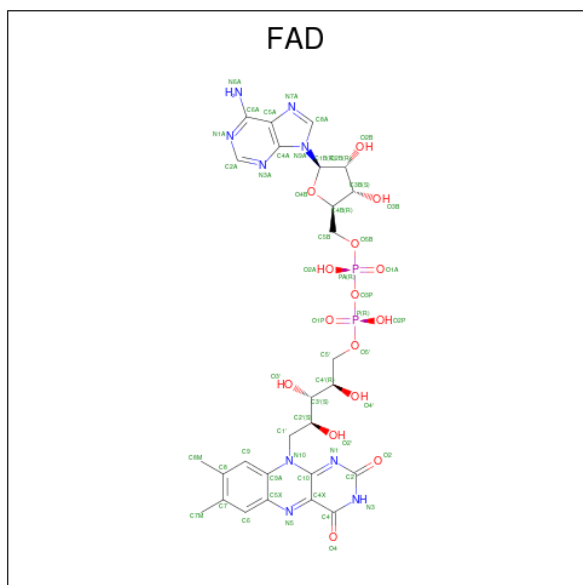
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP O77059
A	-17	ALA	-	expression tag	UNP O77059
A	-16	MET	-	expression tag	UNP O77059
A	-15	GLY	-	expression tag	UNP O77059
A	-14	SER	-	expression tag	UNP O77059
A	-13	GLY	-	expression tag	UNP O77059
A	-12	ILE	-	expression tag	UNP O77059
A	-11	GLN	-	expression tag	UNP O77059
A	-10	ARG	-	expression tag	UNP O77059
A	-9	PRO	-	expression tag	UNP O77059
A	-8	THR	-	expression tag	UNP O77059
A	-7	SER	-	expression tag	UNP O77059
A	-6	THR	-	expression tag	UNP O77059
A	-5	SER	-	expression tag	UNP O77059
A	-4	SER	-	expression tag	UNP O77059
A	-3	LEU	-	expression tag	UNP O77059
A	-2	VAL	-	expression tag	UNP O77059
A	-1	ALA	-	expression tag	UNP O77059
A	0	ALA	-	expression tag	UNP O77059
B	-18	GLY	-	expression tag	UNP O77059
B	-17	ALA	-	expression tag	UNP O77059
B	-16	MET	-	expression tag	UNP O77059
B	-15	GLY	-	expression tag	UNP O77059
B	-14	SER	-	expression tag	UNP O77059
B	-13	GLY	-	expression tag	UNP O77059

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	ILE	-	expression tag	UNP O77059
B	-11	GLN	-	expression tag	UNP O77059
B	-10	ARG	-	expression tag	UNP O77059
B	-9	PRO	-	expression tag	UNP O77059
B	-8	THR	-	expression tag	UNP O77059
B	-7	SER	-	expression tag	UNP O77059
B	-6	THR	-	expression tag	UNP O77059
B	-5	SER	-	expression tag	UNP O77059
B	-4	SER	-	expression tag	UNP O77059
B	-3	LEU	-	expression tag	UNP O77059
B	-2	VAL	-	expression tag	UNP O77059
B	-1	ALA	-	expression tag	UNP O77059
B	0	ALA	-	expression tag	UNP O77059

- 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	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

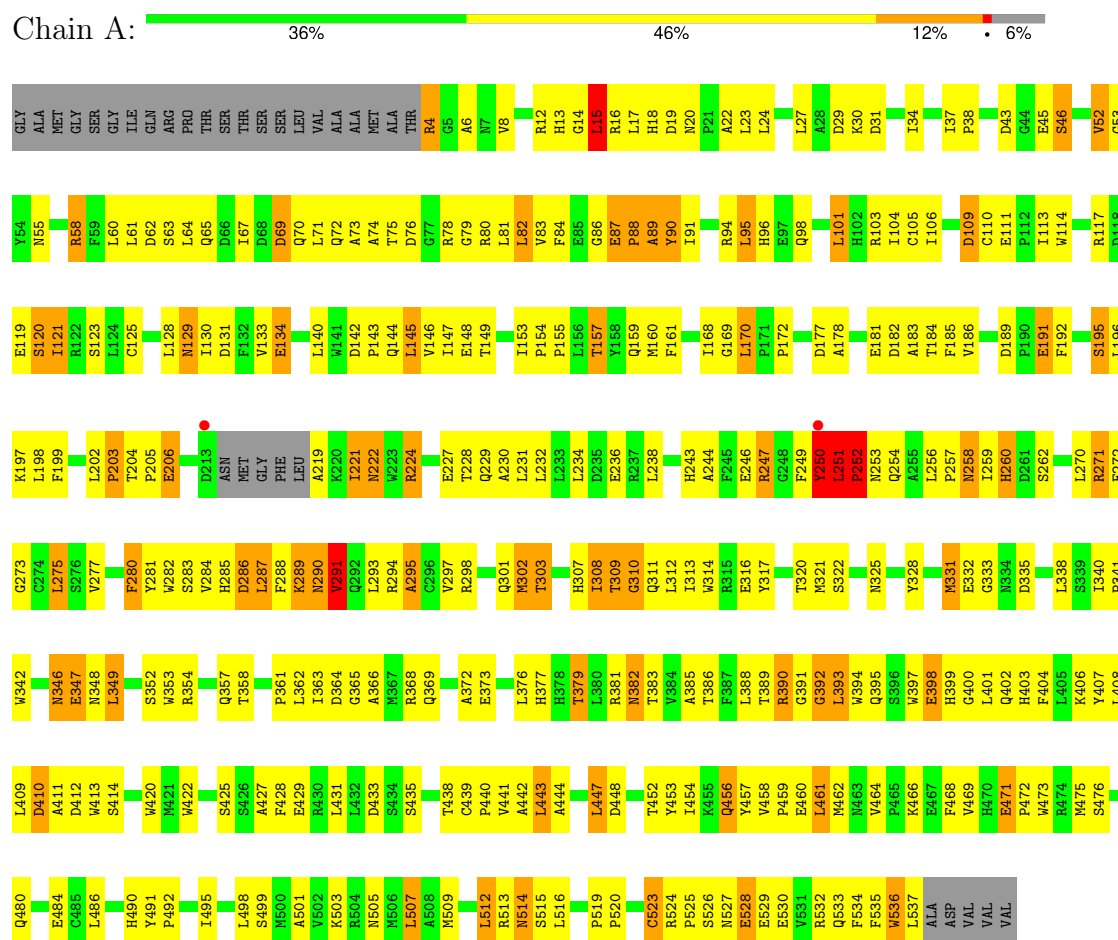
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total 27	O 27	0	0
3	B	25	Total 25	O 25	0	0

3 Residue-property plots

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: Cryptochrome-1



C485	C416	L349	V277	T204	I121
L486	A417	L350	R278	P205	R122
T487	G418	Q351	R279	E206	S123
G488	N419	Q352	F280		L124
N489	W420	W353	Y281	Y211	C125
H490	W421	R354	W282	G212	R126
Y491		L355	S283	D213	E127
P492	A427	G356			L128
E493	F428	Q357	D286	G216	N129
R494	R429	T358	L287	F217	I130
I495	R430	G359	F288	L218	
I496	I431	F360	K289	A219	E134
D497	I432	P361	K280	K220	K135
L498	D433	L362	V291	I221	V136
S499	S434	I363	Q292	N222	S137
M500	S435	D364	L293	W223	H138
	L436	G365		R224	
K503	V437	A366	C296		T149
R504	T438	K367	V297	T228	N150
N505	C439	R368	R298	Q229	G151
M506	P440		G299	A230	G152
L507	W441	L371	V300	L231	I153
A508	A442		Q301	L232	P154
	L443	L376	K302	L233	P155
S511	A444	H377	T303	L234	L156
L512	K445	H378		D235	T157
R513	R446	T379	H307	E236	Y158
N514	L447	L380	T308	R237	Q159
S515	D448		T309	L238	
L516	P449	T383	G310	K239	L162
I517	D450	V384	G311	V240	H163
T518	G451	A385	L312	E241	T164
P519	I452	T386	I313	Q242	V165
P520	Y453	F387		H243	Q166
P521	I454	L388	Y319	A244	L170
H522	I455	T389	T320	F245	P171
C523	D456	K390	M321	F246	P172
R524	Y457	G391	S322	R247	
P525	V458	G392	Y323	G248	T175
S526	P459	L393	N324	F249	A176
N527	E460	W394	N325	Y250	D177
E528	L461	Q395	P326	L251	A178
E529		S396	N327	P252	R179
E530	V464	K397	Y328		L180
V531	P465	E398	D329	L256	E181
R532	K466		R330	P257	
Q533	E467	L401	M331	N258	T184
F534	F468	Q402		I259	F185
F535			N334	H260	V186
W536	E471	L405	D335	D261	
L537	P472	K406	I336	S262	E191
ALA	W473	Y407	C337	P263	F192
ASP	R474	L408	L338		L196
VAL	M475	L409		L270	F199
VAL	S476	D410	W342	R271	L202
VAL	A477	A411	A343	F272	
	E478	D412	K344	G273	
	Q479	W413	P345	C274	
	Q480	S414	N346	L275	
		V415		S276	P203

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.12Å 121.81Å 79.72Å 90.00° 114.78° 90.00°	Depositor
Resolution (Å)	40.49 – 3.20 40.49 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.49-3.20) 99.7 (40.49-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.188 , 0.269 0.185 , 0.264	Depositor DCC
R_{free} test set	1041 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 87.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8746	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.70% 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	0.52	0/4355	0.71	3/5929 (0.1%)
1	B	0.50	0/4469	0.72	1/6082 (0.0%)
All	All	0.51	0/8824	0.72	4/12011 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	LEU	CA-CB-CG	8.68	135.26	115.30
1	A	393	LEU	N-CA-C	6.16	127.62	111.00
1	A	291	VAL	N-CA-C	-5.91	95.03	111.00
1	B	232	LEU	CA-CB-CG	5.01	126.83	115.30

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	4238	0	4076	343	0
1	B	4350	0	4190	342	0
2	A	53	0	31	3	0
2	B	53	0	31	1	0
3	A	27	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	0	1	0
All	All	8746	0	8328	670	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 39.

The worst 5 of 670 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:297:VAL:HG13	1:A:298:ARG:H	0.97	1.09
1:A:297:VAL:HG13	1:A:298:ARG:N	1.79	0.98
1:A:192:PHE:CZ	1:A:196:LEU:HD22	2.04	0.93
1:A:297:VAL:CG1	1:A:298:ARG:H	1.81	0.92
1:A:17:LEU:HD12	1:A:70:GLN:OE1	1.70	0.91

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	525/561 (94%)	409 (78%)	90 (17%)	26 (5%)	1	13
1	B	541/561 (96%)	444 (82%)	70 (13%)	27 (5%)	1	13
All	All	1066/1122 (95%)	853 (80%)	160 (15%)	53 (5%)	1	13

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	221	ILE
1	A	252	PRO

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Mol	Chain	Res	Type
1	A	254	GLN
1	A	291	VAL

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	447/488 (92%)	377 (84%)	70 (16%)	2	10
1	B	458/488 (94%)	384 (84%)	74 (16%)	2	9
All	All	905/976 (93%)	761 (84%)	144 (16%)	2	10

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	303	THR
1	B	535	PHE
1	B	330	ARG
1	B	438	THR
1	A	331	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	55	ASN
1	B	96	HIS
1	B	369	GLN
1	B	301	GLN
1	A	402	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	601	-	54,58,58	0.70	0	71,89,89	1.29	6 (8%)
2	FAD	B	601	-	54,58,58	0.86	1 (1%)	71,89,89	1.24	6 (8%)

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	601	-	-	3/30/50/50	0/6/6/6
2	FAD	B	601	-	-	3/30/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	PA-O3P	4.40	1.64	1.59

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	O3P-PA-O1A	-6.87	90.04	110.70
2	A	601	FAD	O3P-PA-O1A	-5.62	93.78	110.70
2	A	601	FAD	O3P-P-O1P	-3.50	100.18	110.70
2	B	601	FAD	O3P-P-O1P	-3.41	100.43	110.70
2	A	601	FAD	C2'-C1'-N10	3.35	126.03	110.20

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

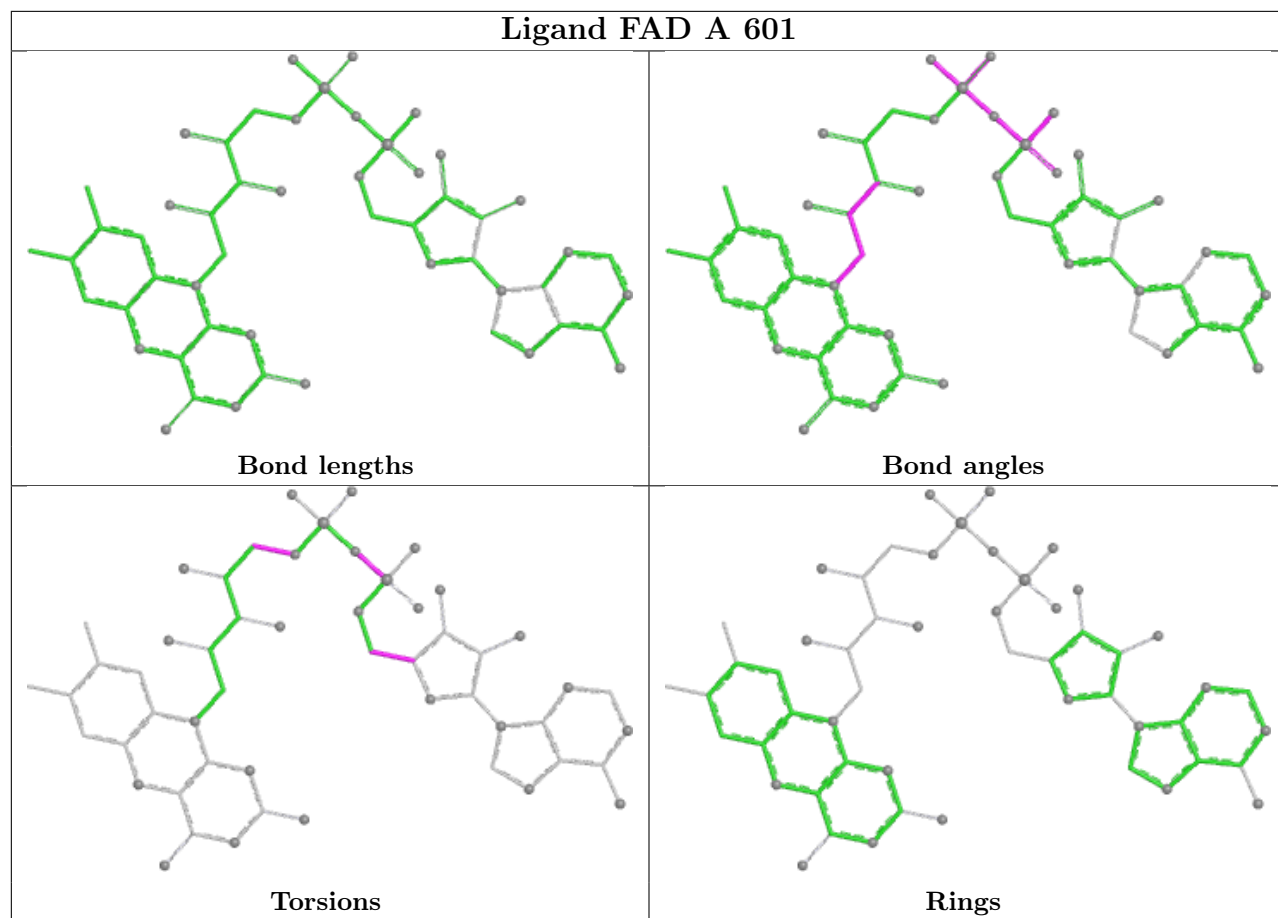
Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C4'-C5'-O5'-P
2	B	601	FAD	C4'-C5'-O5'-P
2	A	601	FAD	P-O3P-PA-O1A
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B

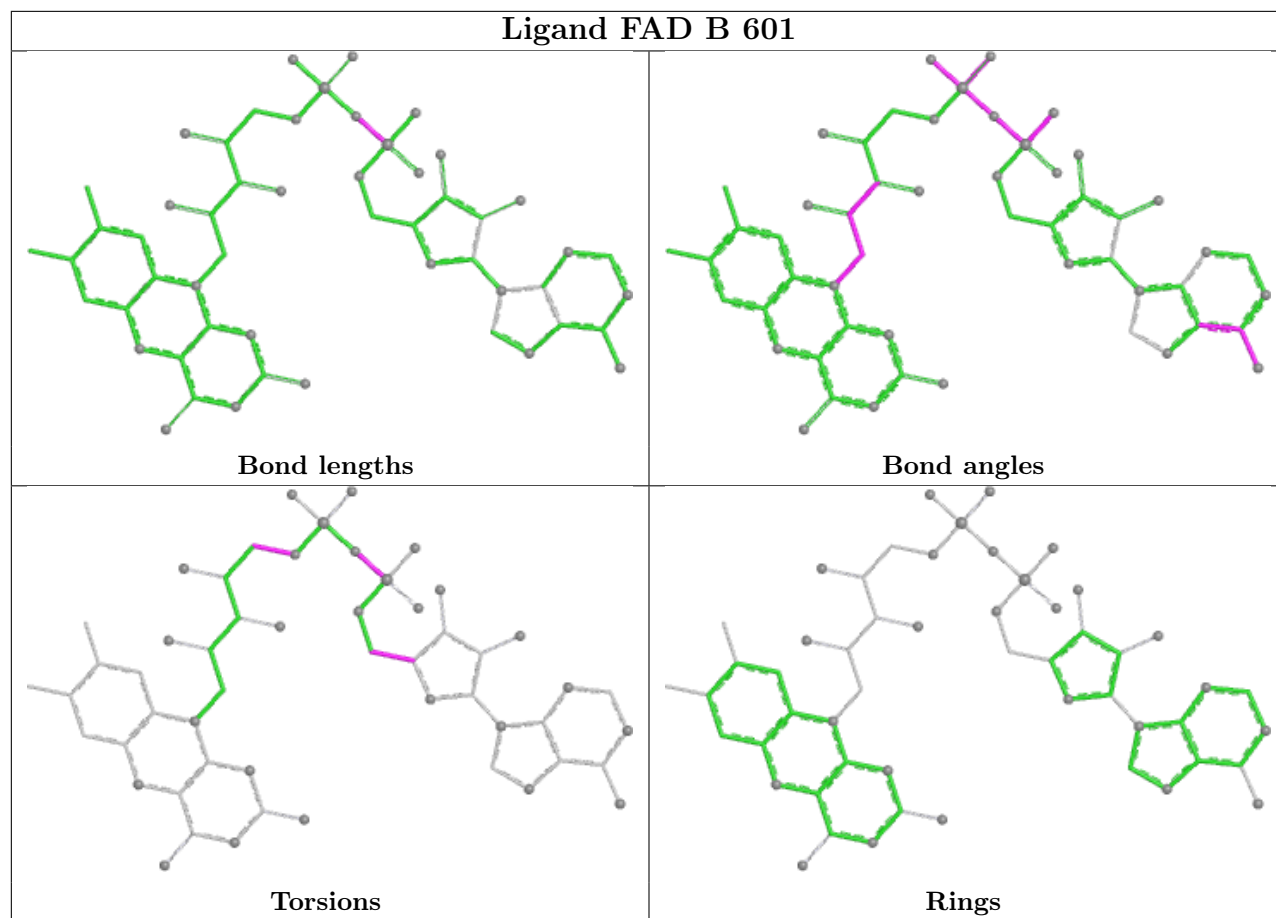
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	3	0
2	B	601	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	529/561 (94%)	-0.59	2 (0%) 89 81	23, 52, 87, 135	0
1	B	543/561 (96%)	-0.54	2 (0%) 89 81	17, 54, 92, 161	0
All	All	1072/1122 (95%)	-0.57	4 (0%) 89 81	17, 54, 90, 161	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	TYR	3.2
1	A	213	ASP	2.5
1	B	218	LEU	2.3
1	B	219	ALA	2.2

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
2	FAD	A	601	53/53	0.97	0.08	37,37,60,60	0

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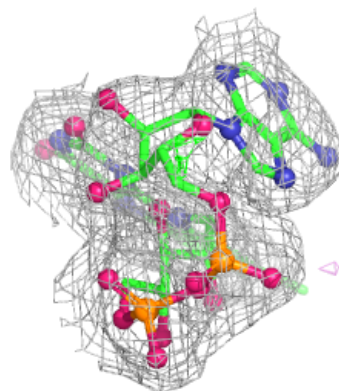
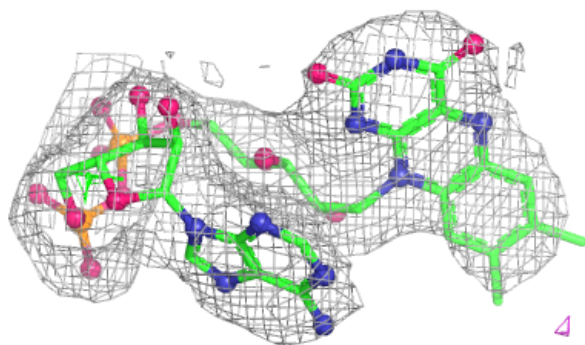
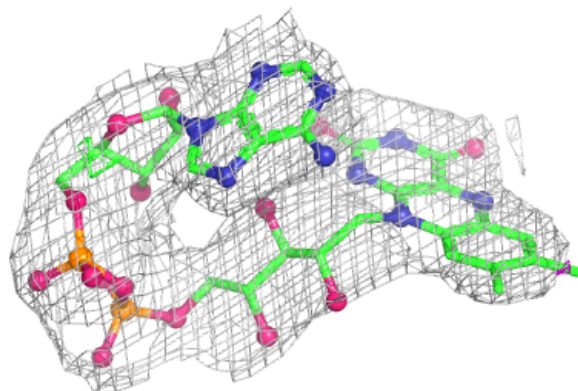
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	B	601	53/53	0.97	0.08	39,39,63,63	0

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.

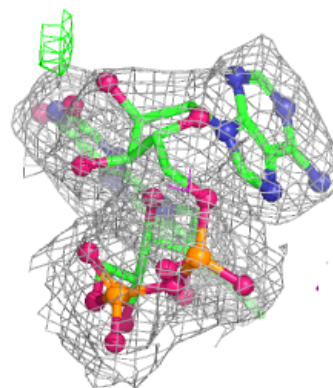
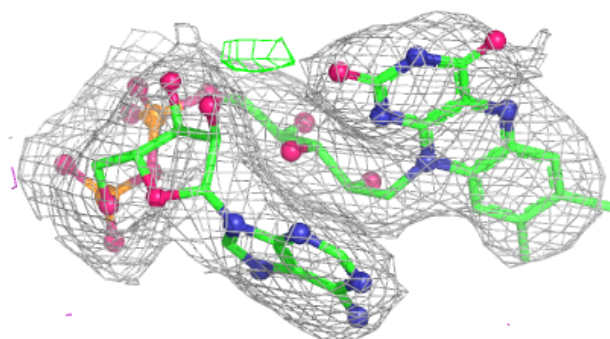
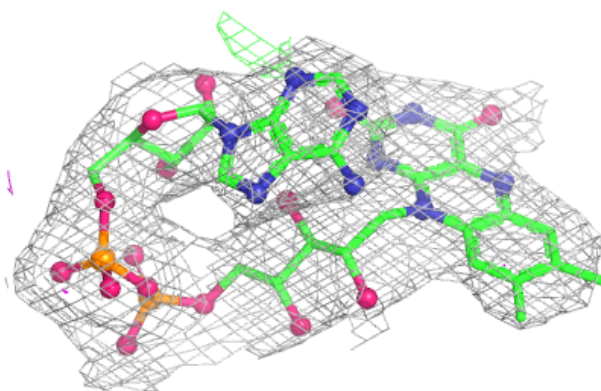
Electron density around FAD A 601:

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 601:

$2mF_o-DF_c$ (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.