



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:12 PM UTC

PDB ID : 4K03 / pdb_00004k03
Title : Crystal structure of Drosophila Cryprochrome
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 : 4-5-2 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

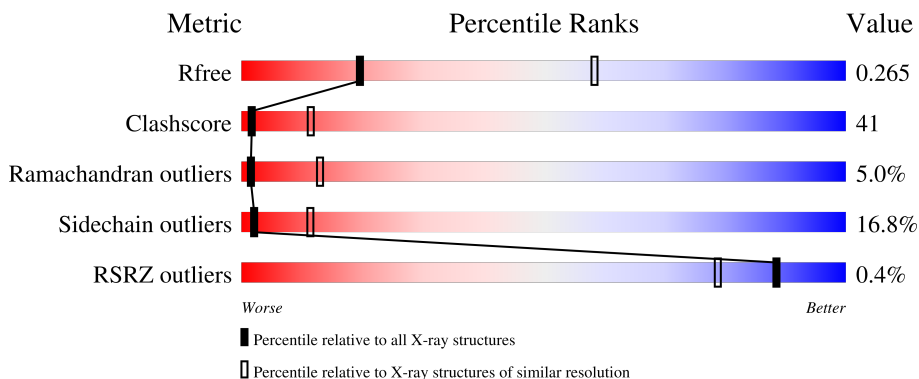
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

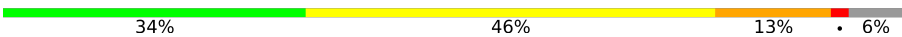
The reported resolution of this entry is 3.20 Å.

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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:

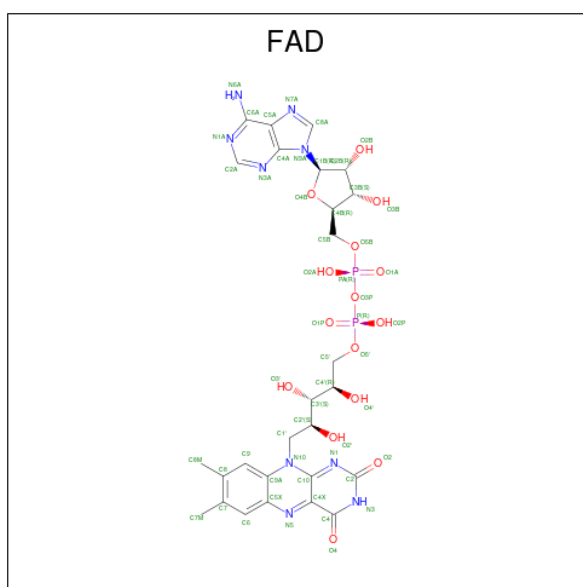
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP O77059
A	-17	ALA	-	expression tag	UNP O77059
A	-16	MET	-	expression tag	UNP O77059
A	-15	GLY	-	expression tag	UNP O77059
A	-14	SER	-	expression tag	UNP O77059
A	-13	GLY	-	expression tag	UNP O77059
A	-12	ILE	-	expression tag	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 (CCD ID: 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	O	0	0
			27	27		

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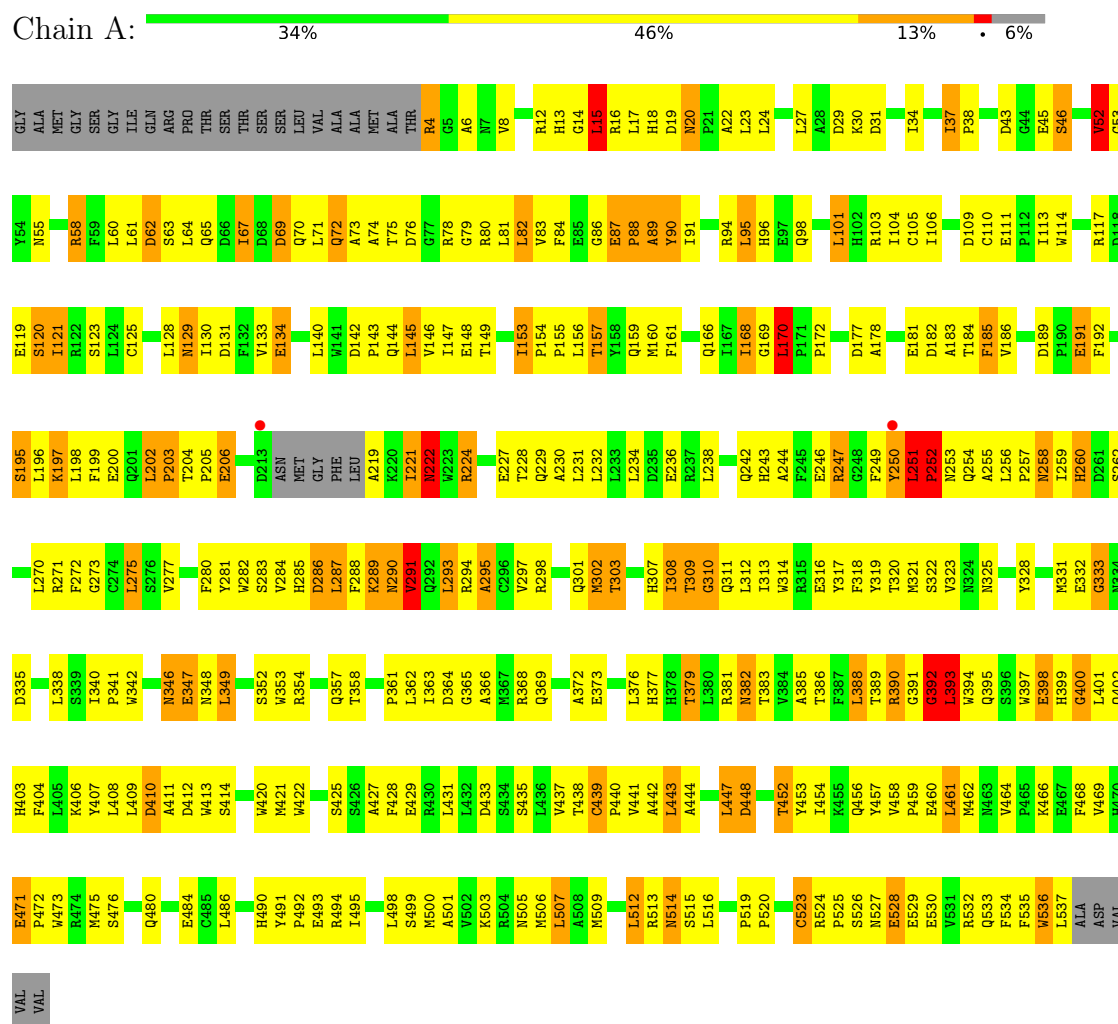
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	25	Total	O	0	0
			25	25		

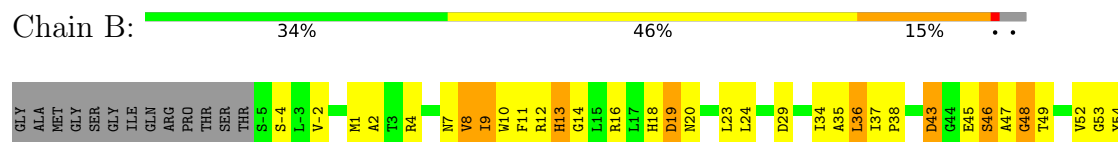
3 Residue-property plots

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



• Molecule 1: Cryptochrome-1



VAL	S476	A477	E478	Q479	Q480	C485	L486	L487	G488	G489	H490	Y491	P492	E493	R494	I495	T496	D497	L498	S499	M500	K503	R504	N505	M506	L507	A508	S511	L512	R513	N514	S515	L516	I517	T518	P519	P520	P521	H522	C523	R524	P525	S526	N527	E528	E529	E530	V531	R532	Q533	F534	F535	M536	L537	ALA	ASP	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
	D410	A411	D412	W413	S414	V415	C416	A417	G418	H419	W420	M421		A427	F428	E429	R430	L431	L432	D433	S434	S435	L436	T437	C438	C439	P440	V441	A442	L443	A444	K445	R446	L447	D448	P449	D450	G451	T452	Y453	L454	R455	Q456	Y457	V458	P459	E460	L461		V464	P465	K466	E467	F468		E471	P472	W473	R474	M475																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
	K344	P345	N346		L349	L350	Q351	S352	K353	R354	L355	G356	Q357	T358	G359	F360	P361	L362	L363	D364	G365	A366	R367	G368	Q369	L370	L371		L376	H377	H378	T379	L380	R381	N382	T383	V384	A385	T386	F387	L388	T389	R390	G391	G392	W393	Q395	S396	R397	E398		L401	Q402		L405	K406	Y407	L408	L409																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
	L275	S276	W277	R278	R279	F280	Y281	W282	S283	R284	H285	D286	L287	F288	K289	N290	V291	Q292	L293		C296	V297	R298	G299	V300	Q301		T303		H307	I308	T309	G310	Q311	L312	I313		Y319	T320	M321	S322	G248	F249	Y250	L251	P252		L256	P257	N258	L259	F332	G333	N334	S262	P263		L336	C337	L338		W342																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
	F199	L202	P203	T204	P205	E206			Y211	G212	D213		G216	F217	L218	A219	K220	L221	N222	W223	R224			T228	Q229	A230				R237	L238	K239	V240	E241	Q242	H243	A244	F245	E246	R247	G248	F249	Y250	L251	P252		L256	P257	N258	L259	H260	D261	S262	P263		L270	R271	F272	G273	C274																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
	R117	D118	E119	S120	I121	R122	L123	L124	C125	R126	L127	L128	M129	I130		E134	K135	V136	S137	H138			T149	N150	G151	G152	I153	P154	P155	L156	T157	G158	Y158	Q159		L162	H163	T164	V165	Q166		L170	P171	P172		T175	A176	D177	A178	R179	L180	E181		T184	F185	V186		E191	F192		L196																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														

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 0.186 , 0.265	Depositor DCC
R_{free} test set	1041 reflections (5.10%)	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	0.64	0/4355	1.07	30/5929 (0.5%)
1	B	0.64	0/4469	1.12	30/6082 (0.5%)
All	All	0.64	0/8824	1.09	60/12011 (0.5%)

There are no bond length outliers.

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	CYS	CA-C-N	12.86	132.63	119.64
1	B	439	CYS	C-N-CA	12.86	132.63	119.64
1	A	20	ASN	CA-C-N	11.86	132.21	119.05
1	A	20	ASN	C-N-CA	11.86	132.21	119.05
1	B	20	ASN	CA-C-N	9.81	129.94	119.05

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	355	0
1	B	4350	0	4190	362	0
2	A	53	0	31	3	0
2	B	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	0	1	0
3	B	25	0	0	1	0
All	All	8746	0	8328	703	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 41.

The worst 5 of 703 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: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
1:A:297:VAL:HG13	1:A:298:ARG:N	1.79	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

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Mol	Chain	Res	Type
1	A	252	PRO
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%)	375 (84%)	72 (16%)	2	13
1	B	458/488 (94%)	378 (82%)	80 (18%)	2	10
All	All	905/976 (93%)	753 (83%)	152 (17%)	2	11

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	283	SER
1	B	487	ILE
1	B	300	VAL
1	B	379	THR
1	B	517	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	301	GLN
1	B	369	GLN
1	A	505	ASN
1	A	533	GLN
1	B	32	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	58,58,58	0.49	0	85,89,89	1.14	6 (7%)
2	FAD	B	601	-	58,58,58	0.72	1 (1%)	85,89,89	1.08	5 (5%)

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	-	-	3/34/50/50	0/6/6/6
2	FAD	B	601	-	-	3/34/50/50	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 11 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:

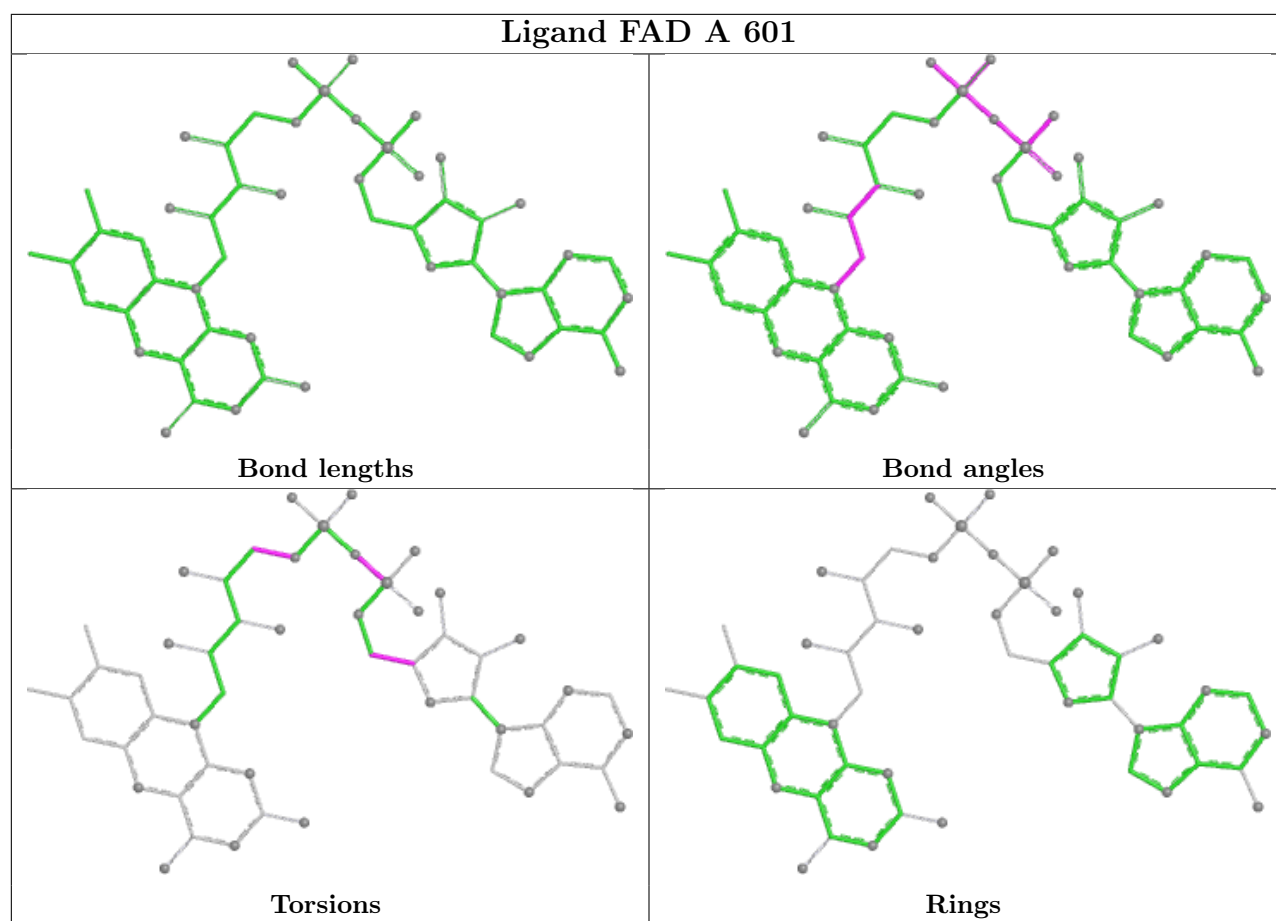
Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C4'-C5'-O5'-P
2	B	601	FAD	C4'-C5'-O5'-P
2	A	601	FAD	P-O3P-PA-O1A
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B

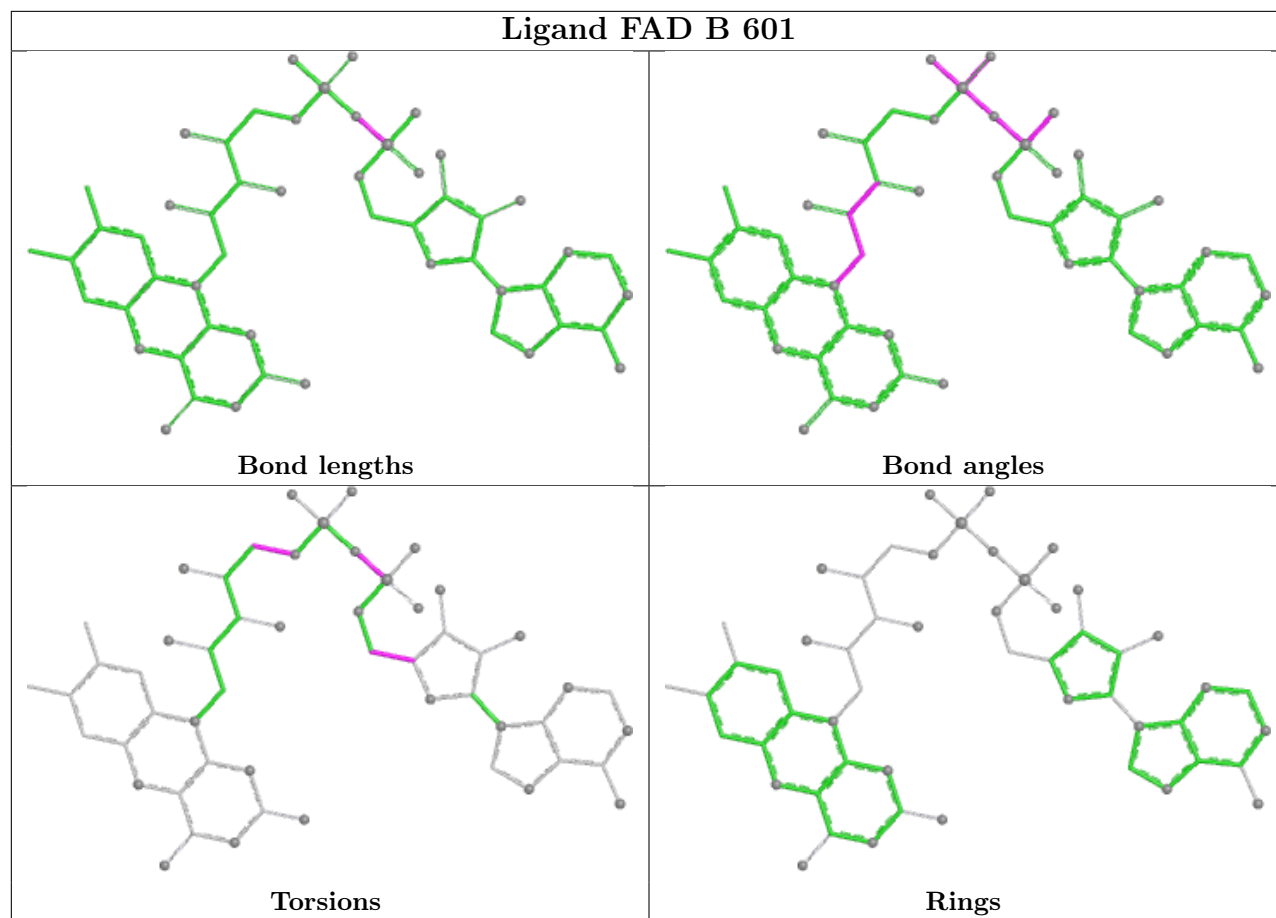
There are no ring outliers.

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%)	-0.44	2 (0%) 88 79	23, 52, 87, 135	0
1	B	543/561 (96%)	-0.39	2 (0%) 88 79	17, 54, 92, 161	0
All	All	1072/1122 (95%)	-0.42	4 (0%) 88 79	17, 54, 90, 161	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	TYR	3.4
1	A	213	ASP	2.7
1	B	218	LEU	2.5
1	B	219	ALA	2.3

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

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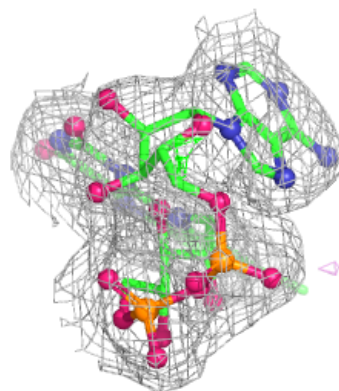
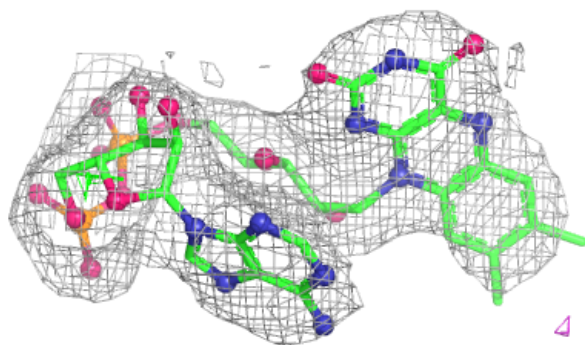
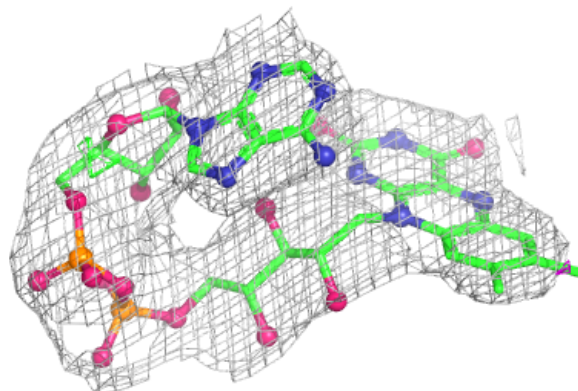
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	601	53/53	0.97	0.08	39,39,63,63	0

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.

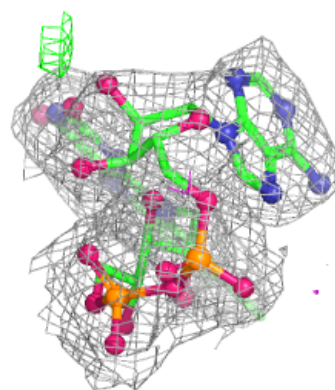
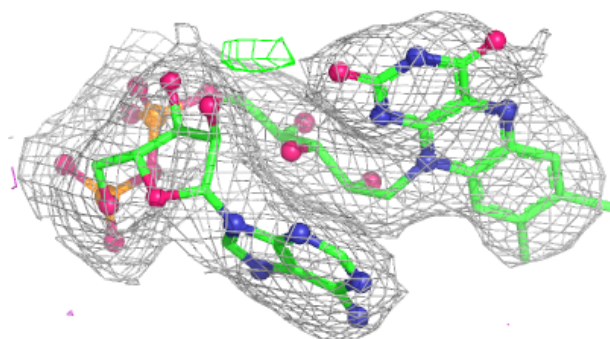
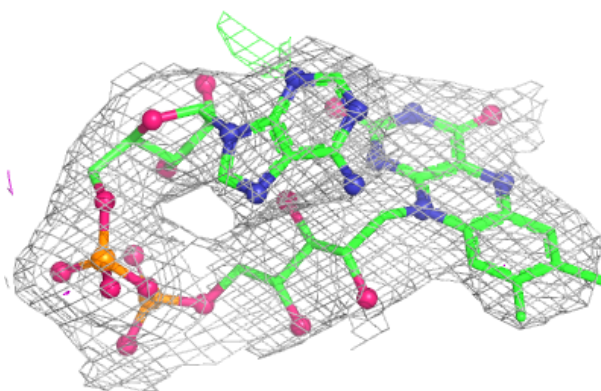
Electron density around FAD A 601:

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.