



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:45 am GMT

PDB ID : 4I6E
Title : A vertebrate cryptochrome
Authors : Xing, W.; Busino, L.; Hinds, T.R.; Marionni, S.T.; Saifee, N.H.; Bush, M.F.;
Pagano, M.; Zheng, N.
Deposited on : 2012-11-29
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

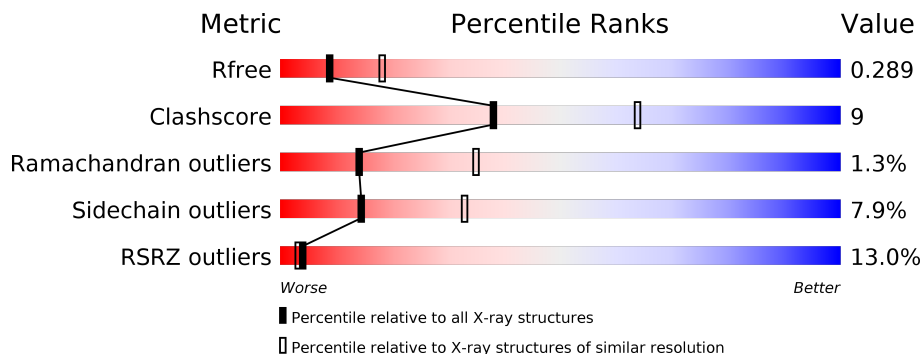
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	512	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3822 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3821	2460	669	673	19			

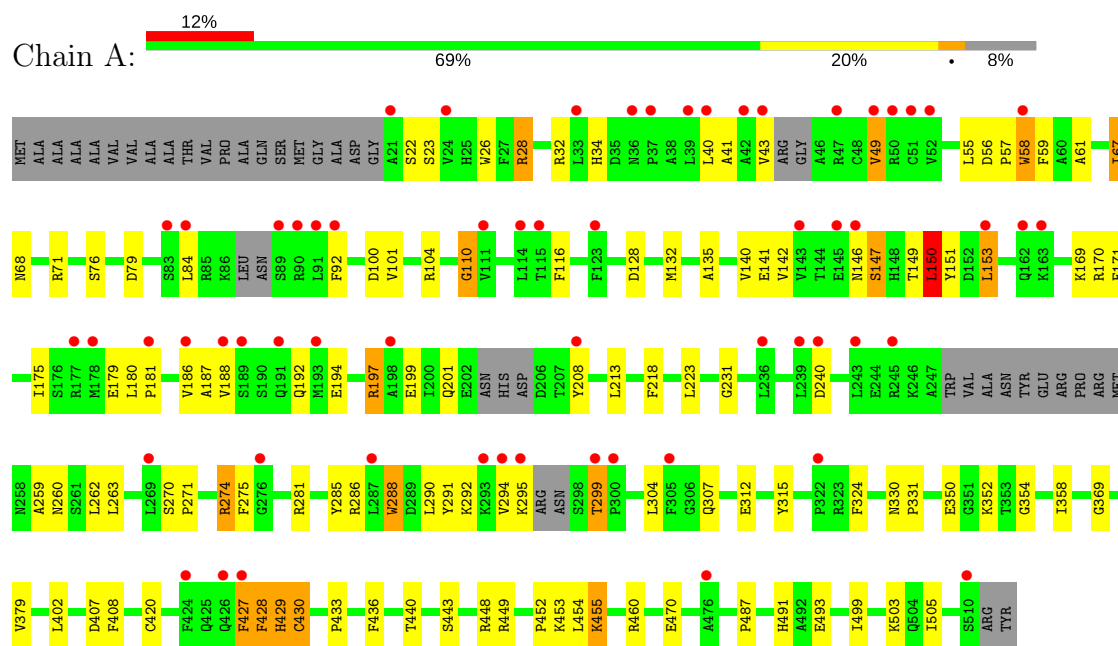
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	68.94Å 68.94Å 127.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.70 48.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.74-2.70) 99.9 (48.74-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.244 , 0.287 0.245 , 0.289	Depositor DCC
R_{free} test set	1377 reflections (8.41%)	DCC
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3822	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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

5.1 Standard geometry

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	0.44	0/3928	0.64	1/5323 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	LEU	CA-CB-CG	5.11	127.04	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3821	0	3757	66	0
2	A	1	0	0	0	0
All	All	3822	0	3757	66	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 9.

All (66) 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:428:PHE:HA	1:A:429:HIS:HB2	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:GLY:HA3	1:A:487:PRO:HA	1.70	0.72
1:A:150:LEU:N	1:A:312:GLU:OE2	2.23	0.70
1:A:194:GLU:HA	1:A:197:ARG:HE	1.61	0.66
1:A:199:GLU:OE1	1:A:201:GLN:NE2	2.29	0.66
1:A:443:SER:O	1:A:448:ARG:NH2	2.28	0.66
1:A:132:MET:HG2	1:A:142:VAL:HG11	1.79	0.63
1:A:194:GLU:HB3	1:A:197:ARG:HH21	1.64	0.63
1:A:259:ALA:HA	1:A:262:LEU:HD23	1.81	0.62
1:A:436:PHE:O	1:A:440:THR:HG23	1.99	0.61
1:A:56:ASP:HB3	1:A:59:PHE:HB3	1.82	0.61
1:A:23:SER:HB2	1:A:49:VAL:HG23	1.85	0.59
1:A:149:THR:HG21	1:A:153:LEU:HD21	1.85	0.59
1:A:171:PHE:O	1:A:175:ILE:HG12	2.04	0.57
1:A:354:GLY:HA3	1:A:487:PRO:CA	2.34	0.56
1:A:40:LEU:HD23	1:A:188:VAL:HG12	1.88	0.55
1:A:34:HIS:HA	1:A:187:ALA:HB2	1.89	0.55
1:A:194:GLU:HA	1:A:197:ARG:NE	2.21	0.55
1:A:58:TRP:HA	1:A:61:ALA:HB3	1.90	0.53
1:A:429:HIS:O	1:A:430:CYS:HB2	2.08	0.53
1:A:448:ARG:HG2	1:A:455:LYS:HA	1.92	0.52
1:A:433:PRO:HD3	1:A:491:HIS:CE1	2.45	0.51
1:A:26:TRP:CD2	1:A:28:ARG:HD2	2.46	0.51
1:A:67:ILE:HG23	1:A:218:PHE:CD2	2.46	0.51
1:A:420:CYS:SG	1:A:427:PHE:HA	2.50	0.51
1:A:428:PHE:HA	1:A:429:HIS:CB	2.31	0.50
1:A:146:ASN:O	1:A:281:ARG:NH2	2.43	0.50
1:A:240:ASP:OD2	1:A:286:ARG:NH2	2.45	0.50
1:A:291:TYR:CE2	1:A:295:LYS:HD2	2.48	0.49
1:A:315:TYR:OH	1:A:407:ASP:OD1	2.09	0.47
1:A:26:TRP:HB3	1:A:116:PHE:HB3	1.97	0.47
1:A:135:ALA:HB1	1:A:140:VAL:HB	1.96	0.47
1:A:32:ARG:NH2	1:A:147:SER:HB2	2.29	0.47
1:A:101:VAL:HG22	1:A:104:ARG:HH21	1.80	0.47
1:A:56:ASP:HA	1:A:57:PRO:HD3	1.79	0.47
1:A:76:SER:HA	1:A:231:GLY:HA2	1.98	0.46
1:A:201:GLN:OE1	1:A:201:GLN:N	2.47	0.46
1:A:350:GLU:HB3	1:A:352:LYS:HE3	1.97	0.46
1:A:151:TYR:OH	1:A:175:ILE:HG23	2.17	0.45
1:A:175:ILE:HD13	1:A:175:ILE:HA	1.81	0.45
1:A:292:LYS:HD3	1:A:292:LYS:O	2.16	0.45
1:A:67:ILE:HD12	1:A:68:ASN:H	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:SER:OG	1:A:22:SER:O	2.35	0.45
1:A:151:TYR:CZ	1:A:181:PRO:HG3	2.52	0.45
1:A:324:PHE:HB3	1:A:408:PHE:CZ	2.52	0.44
1:A:179:GLU:H	1:A:179:GLU:CD	2.20	0.44
1:A:288:TRP:HZ2	1:A:299:THR:HG22	1.83	0.44
1:A:128:ASP:O	1:A:132:MET:HG3	2.18	0.43
1:A:181:PRO:O	1:A:285:TYR:OH	2.23	0.43
1:A:452:PRO:C	1:A:454:LEU:H	2.21	0.43
1:A:67:ILE:H	1:A:67:ILE:HG13	1.48	0.43
1:A:71:ARG:HD3	1:A:213:LEU:HD11	1.99	0.43
1:A:499:ILE:HA	1:A:499:ILE:HD13	1.83	0.42
1:A:330:ASN:HA	1:A:331:PRO:HD3	1.94	0.42
1:A:213:LEU:O	1:A:218:PHE:HB2	2.19	0.42
1:A:84:LEU:HA	1:A:84:LEU:HD23	1.91	0.42
1:A:274:ARG:HD3	1:A:275:PHE:CD1	2.55	0.42
1:A:92:PHE:HA	1:A:208:TYR:HB3	2.01	0.42
1:A:270:SER:OG	1:A:271:PRO:HD3	2.19	0.41
1:A:358:ILE:HG23	1:A:379:VAL:HG12	2.02	0.41
1:A:369:GLY:HA2	1:A:402:LEU:O	2.20	0.41
1:A:43:VAL:HG12	1:A:192:GLN:NE2	2.35	0.41
1:A:22:SER:OG	1:A:110:GLY:O	2.30	0.41
1:A:290:LEU:O	1:A:294:VAL:HG23	2.20	0.41
1:A:43:VAL:HG12	1:A:192:GLN:HE21	1.86	0.41
1:A:150:LEU:HB2	1:A:312:GLU:OE2	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	459/512 (90%)	410 (89%)	43 (9%)	6 (1%)	14 35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	HIS
1	A	430	CYS
1	A	41	ALA
1	A	100	ASP
1	A	197	ARG
1	A	110	GLY

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	404/434 (93%)	372 (92%)	32 (8%)	14	33

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	49	VAL
1	A	55	LEU
1	A	58	TRP
1	A	67	ILE
1	A	79	ASP
1	A	141	GLU
1	A	147	SER
1	A	150	LEU
1	A	153	LEU
1	A	169	LYS
1	A	170	ARG
1	A	180	LEU
1	A	186	VAL
1	A	223	LEU
1	A	260	ASN
1	A	263	LEU
1	A	274	ARG
1	A	288	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	299	THR
1	A	304	LEU
1	A	307	GLN
1	A	427	PHE
1	A	428	PHE
1	A	449	ARG
1	A	453	LYS
1	A	455	LYS
1	A	460	ARG
1	A	470	GLU
1	A	493	GLU
1	A	503	LYS
1	A	505	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	471/512 (91%)	0.75	61 (12%) 4 3	43, 110, 168, 201	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	VAL	7.9
1	A	33	LEU	7.6
1	A	245	ARG	7.0
1	A	193	MET	6.1
1	A	143	VAL	5.8
1	A	111	VAL	5.7
1	A	424	PHE	5.7
1	A	39	LEU	5.5
1	A	188	VAL	5.1
1	A	92	PHE	5.0
1	A	177	ARG	4.8
1	A	89	SER	4.6
1	A	191	GLN	4.5
1	A	186	VAL	4.5
1	A	36	ASN	4.4
1	A	269	LEU	4.4
1	A	51	CYS	4.2
1	A	91	LEU	4.1
1	A	510	SER	4.0
1	A	47	ARG	3.9
1	A	153	LEU	3.8
1	A	243	LEU	3.8
1	A	83	SER	3.7
1	A	21	ALA	3.6
1	A	300	PRO	3.6
1	A	49	VAL	3.5
1	A	240	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	236	LEU	3.3
1	A	293	LYS	3.2
1	A	84	LEU	3.1
1	A	198	ALA	3.0
1	A	189	SER	3.0
1	A	305	PHE	3.0
1	A	114	LEU	3.0
1	A	40	LEU	2.9
1	A	162	GLN	2.8
1	A	178	MET	2.7
1	A	115	THR	2.7
1	A	50	ARG	2.7
1	A	427	PHE	2.7
1	A	299	THR	2.7
1	A	163	LYS	2.7
1	A	37	PRO	2.6
1	A	208	TYR	2.6
1	A	146	ASN	2.5
1	A	476	ALA	2.5
1	A	145	GLU	2.5
1	A	42	ALA	2.4
1	A	43	VAL	2.4
1	A	52	VAL	2.4
1	A	426	GLN	2.3
1	A	276	GLY	2.3
1	A	295	LYS	2.3
1	A	322	PRO	2.2
1	A	181	PRO	2.2
1	A	58	TRP	2.2
1	A	123	PHE	2.1
1	A	239	LEU	2.1
1	A	294	VAL	2.0
1	A	287	LEU	2.0
1	A	90	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.