



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:19 PM GMT

PDB ID : 4K0R
Title : Crystal structure of mouse Cryptochrome 1
Authors : Czarna, A.; Wolf, E.
Deposited on : 2013-04-04
Resolution : 2.65 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

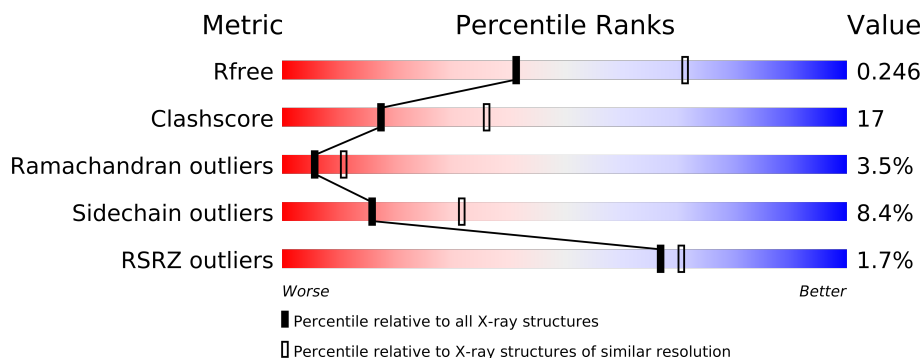
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.65 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}	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	617	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3693 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			Total	C	N	O	S			
1	A	463	3622	2332	626	643	21	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	607	ALA	-	EXPRESSION TAG	UNP P97784
A	608	ALA	-	EXPRESSION TAG	UNP P97784
A	609	ALA	-	EXPRESSION TAG	UNP P97784
A	610	LEU	-	EXPRESSION TAG	UNP P97784
A	611	GLU	-	EXPRESSION TAG	UNP P97784
A	612	HIS	-	EXPRESSION TAG	UNP P97784
A	613	HIS	-	EXPRESSION TAG	UNP P97784
A	614	HIS	-	EXPRESSION TAG	UNP P97784
A	615	HIS	-	EXPRESSION TAG	UNP P97784
A	616	HIS	-	EXPRESSION TAG	UNP P97784
A	617	HIS	-	EXPRESSION TAG	UNP P97784

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	71	Total	O	0	0
			71	71		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.17Å 79.55Å 127.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.73 – 2.65 41.73 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.73-2.65) 99.8 (41.73-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.190 , 0.260 0.184 , 0.246	Depositor DCC
R_{free} test set	682 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 13625 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3693	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.49	0/3721	0.63	0/5068

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	ASP	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3622	0	3459	123	0
2	A	71	0	0	9	0
All	All	3693	0	3459	123	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (123) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:162:PRO:C	1:A:163:LEU:HG	1.42	1.16
1:A:200:PHE:HB3	1:A:201:ASP:HB2	1.29	1.12
1:A:185:ASP:O	1:A:187:ASP:N	1.84	1.07
1:A:162:PRO:C	1:A:163:LEU:CG	2.33	0.97
1:A:232:ALA:HB1	1:A:277:LYS:HE2	1.51	0.92
1:A:402:CYS:HB2	2:A:766:HOH:O	1.70	0.92
1:A:359:HIS:CD2	1:A:400:LEU:HD11	2.06	0.91
1:A:200:PHE:CB	1:A:201:ASP:HB2	2.01	0.89
1:A:461:LEU:H	1:A:465:ASN:HD22	1.17	0.89
1:A:162:PRO:O	1:A:163:LEU:HG	1.71	0.88
1:A:341:ASP:O	1:A:345:THR:HG23	1.74	0.87
1:A:274:LYS:HG2	1:A:280:SER:HA	1.57	0.86
1:A:196:GLU:HA	1:A:200:PHE:O	1.79	0.81
1:A:72:ARG:HD3	1:A:185:ASP:OD2	1.79	0.80
1:A:232:ALA:CB	1:A:277:LYS:HE2	2.13	0.79
1:A:461:LEU:H	1:A:465:ASN:ND2	1.82	0.78
1:A:484:MET:HE3	2:A:766:HOH:O	1.85	0.76
1:A:281:SER:HB3	2:A:759:HOH:O	1.85	0.75
1:A:202:THR:HB	1:A:205:LEU:N	2.03	0.73
1:A:165:MET:HB3	1:A:166:PRO:CD	2.21	0.71
1:A:461:LEU:N	1:A:465:ASN:HD22	1.88	0.70
1:A:244:LEU:HD11	1:A:339:TRP:HH2	1.56	0.70
1:A:343:ILE:HG12	1:A:357:ALA:HB1	1.74	0.70
1:A:131:THR:HB	1:A:294:GLU:OE2	1.92	0.69
1:A:186:HIS:O	1:A:187:ASP:HB3	1.93	0.69
1:A:162:PRO:O	1:A:163:LEU:CG	2.39	0.67
1:A:132:LEU:N	1:A:294:GLU:OE2	2.25	0.66
1:A:200:PHE:CA	1:A:201:ASP:HB2	2.26	0.65
1:A:355:HIS:HD2	2:A:716:HOH:O	1.81	0.64
1:A:183:SER:OG	1:A:184:ASP:N	2.29	0.64
1:A:200:PHE:HB3	1:A:201:ASP:CB	2.19	0.63
1:A:487:ILE:HG22	1:A:487:ILE:O	1.97	0.62
1:A:165:MET:CB	1:A:166:PRO:CD	2.75	0.62
1:A:207:SER:O	1:A:208:ALA:CB	2.49	0.60
1:A:487:ILE:O	1:A:487:ILE:CG2	2.49	0.60
1:A:157:VAL:HA	1:A:160:MET:HG3	1.82	0.60
1:A:284:LEU:HD22	1:A:291:LEU:HD11	1.84	0.58
1:A:162:PRO:CA	1:A:163:LEU:HG	2.29	0.58
1:A:165:MET:HB3	1:A:166:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:89:LYS:HD3	1:A:90:GLU:OE2	2.04	0.58
1:A:477:SER:O	1:A:481:ILE:HG13	2.04	0.57
1:A:86:ARG:O	1:A:90:GLU:HG2	2.04	0.57
1:A:165:MET:HB3	1:A:166:PRO:HD3	1.87	0.56
1:A:244:LEU:HD11	1:A:339:TRP:CH2	2.39	0.56
1:A:71:SER:OG	1:A:180:THR:HG21	2.05	0.56
1:A:138:ILE:HG23	1:A:156:LEU:HD22	1.88	0.56
1:A:415:PRO:HD2	1:A:473:HIS:NE2	2.23	0.54
1:A:47:VAL:HA	1:A:383:GLU:HG2	1.89	0.54
1:A:303:ASN:O	1:A:306:PHE:HB2	2.08	0.54
1:A:162:PRO:O	1:A:163:LEU:CD2	2.57	0.53
1:A:273:TYR:CD2	1:A:282:PRO:HB3	2.44	0.53
1:A:57:GLN:O	1:A:61:ASP:HB2	2.09	0.53
1:A:367:ARG:HD3	2:A:766:HOH:O	2.08	0.52
1:A:466:TYR:CG	1:A:467:PRO:HD2	2.45	0.52
1:A:448:TRP:CE3	1:A:469:PRO:HG3	2.45	0.51
1:A:60:GLU:OE2	1:A:192:VAL:HB	2.10	0.51
1:A:47:VAL:HG13	1:A:52:TRP:HE1	1.76	0.51
1:A:149:THR:HG22	1:A:152:ARG:H	1.76	0.51
1:A:270:THR:CG2	1:A:274:LYS:HE3	2.40	0.51
1:A:164:GLU:O	1:A:165:MET:O	2.29	0.51
1:A:165:MET:O	1:A:166:PRO:O	2.29	0.51
1:A:126:VAL:O	1:A:127:ARG:HD3	2.11	0.51
1:A:164:GLU:O	1:A:165:MET:C	2.50	0.50
1:A:141:LEU:HD12	1:A:156:LEU:HD21	1.93	0.50
1:A:252:SER:OG	1:A:253:PRO:HD3	2.11	0.50
1:A:25:ILE:CG1	1:A:31:ILE:HD12	2.42	0.50
1:A:104:PRO:HD2	1:A:390:TRP:CZ3	2.47	0.49
1:A:466:TYR:CD1	1:A:467:PRO:HD2	2.48	0.49
1:A:107:LYS:HE3	1:A:301:THR:OG1	2.13	0.49
1:A:22:LYS:O	1:A:26:GLN:HG2	2.13	0.48
1:A:37:LEU:CD1	1:A:193:PRO:HG3	2.43	0.48
1:A:305:ARG:HD2	1:A:311:GLY:O	2.14	0.48
1:A:279:ASN:OD1	1:A:279:ASN:C	2.52	0.48
1:A:445:TYR:HB2	2:A:720:HOH:O	2.13	0.47
1:A:369:ASP:OD2	2:A:767:HOH:O	2.20	0.47
1:A:481:ILE:O	1:A:485:LYS:HG2	2.15	0.47
1:A:142:ASN:HB3	1:A:145:GLN:O	2.15	0.47
1:A:245:LEU:HD21	1:A:431:ARG:HD3	1.96	0.47
1:A:308:LYS:HB2	1:A:308:LYS:HE2	1.69	0.47
1:A:396:SER:O	1:A:400:LEU:HB2	2.15	0.46
1:A:190:TYR:N	1:A:190:TYR:CD1	2.82	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:112:ALA:O	1:A:116:LEU:HD13	2.16	0.46
1:A:165:MET:CB	1:A:166:PRO:HD2	2.42	0.46
1:A:405:PHE:O	1:A:406:PHE:C	2.54	0.46
1:A:358:ARG:NH1	1:A:385:LEU:HD11	2.31	0.45
1:A:265:PHE:HD2	1:A:290:LEU:HD21	1.81	0.45
1:A:323:ASN:HB3	1:A:372:ILE:HD11	1.99	0.45
1:A:256:ARG:HD2	1:A:256:ARG:O	2.17	0.45
1:A:187:ASP:OD1	1:A:187:ASP:C	2.54	0.45
1:A:306:PHE:HB3	1:A:390:TRP:CH2	2.52	0.44
1:A:362:ALA:HA	1:A:397:TRP:CH2	2.51	0.44
1:A:162:PRO:O	1:A:163:LEU:HD23	2.17	0.44
1:A:161:GLU:HA	1:A:162:PRO:HD3	1.73	0.44
1:A:367:ARG:HH22	1:A:411:HIS:N	2.16	0.44
1:A:129:SER:HA	1:A:263:ARG:CZ	2.48	0.44
1:A:415:PRO:CD	1:A:473:HIS:CE1	3.00	0.44
1:A:152:ARG:HD2	1:A:152:ARG:HA	1.57	0.44
1:A:444:ILE:O	1:A:444:ILE:HG13	2.18	0.44
1:A:32:ARG:HD3	1:A:91:TRP:CZ3	2.53	0.43
1:A:351:GLY:HA2	1:A:384:LEU:O	2.18	0.43
1:A:61:ASP:OD2	1:A:213:GLY:HA3	2.18	0.43
1:A:109:ARG:NE	1:A:110:ASP:OD1	2.49	0.43
1:A:72:ARG:HG2	1:A:182:LEU:CD2	2.49	0.43
1:A:69:LEU:O	1:A:70:ASN:HB2	2.18	0.43
1:A:272:LEU:CD2	2:A:758:HOH:O	2.67	0.42
1:A:160:MET:HB3	1:A:160:MET:HE2	1.94	0.42
1:A:180:THR:HA	1:A:181:PRO:HD3	1.49	0.42
1:A:68:LYS:HB3	1:A:68:LYS:HE2	1.62	0.42
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.85	0.41
1:A:4:ASN:HB2	1:A:92:ASN:O	2.19	0.41
1:A:25:ILE:HG12	1:A:31:ILE:HD12	2.01	0.41
1:A:56:LEU:HD13	1:A:193:PRO:O	2.20	0.41
1:A:20:ALA:HB2	1:A:127:ARG:HB2	2.02	0.41
1:A:23:GLU:O	1:A:26:GLN:HB2	2.20	0.41
1:A:38:ASP:HA	1:A:39:PRO:HD3	1.85	0.41
1:A:274:LYS:HE2	1:A:280:SER:O	2.20	0.41
1:A:65:ASN:O	1:A:68:LYS:HB2	2.21	0.41
1:A:6:VAL:HG23	1:A:93:ILE:HD12	2.02	0.41
1:A:9:PHE:HE2	1:A:33:CYS:HB3	1.86	0.41
1:A:23:GLU:OE1	1:A:127:ARG:NE	2.54	0.40
1:A:357:ALA:O	1:A:361:VAL:HG22	2.21	0.40
1:A:420:ARG:NE	2:A:770:HOH:O	2.32	0.40
1:A:3:VAL:HG22	1:A:29:ASP:OD1	2.22	0.40

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	453/617 (73%)	405 (89%)	32 (7%)	16 (4%)	6	11

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	PRO
1	A	186	HIS
1	A	187	ASP
1	A	201	ASP
1	A	207	SER
1	A	208	ALA
1	A	234	PHE
1	A	236	ARG
1	A	406	PHE
1	A	407	GLN
1	A	129	SER
1	A	235	GLU
1	A	408	GLN
1	A	142	ASN
1	A	411	HIS
1	A	165	MET

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	368/521 (71%)	337 (92%)	31 (8%)	16	32

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ILE
1	A	47	VAL
1	A	51	ARG
1	A	69	LEU
1	A	72	ARG
1	A	76	ILE
1	A	145	GLN
1	A	152	ARG
1	A	160	MET
1	A	163	LEU
1	A	164	GLU
1	A	165	MET
1	A	180	THR
1	A	182	LEU
1	A	187	ASP
1	A	202	THR
1	A	247	SER
1	A	272	LEU
1	A	285	SER
1	A	286	LEU
1	A	308	LYS
1	A	327	LEU
1	A	345	THR
1	A	385	LEU
1	A	387	ASP
1	A	400	LEU
1	A	420	ARG
1	A	431	ARG
1	A	444	ILE
1	A	459	LYS
1	A	471	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	GLN
1	A	359	HIS
1	A	465	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	463/617 (75%)	-0.15	8 (1%) 67 71	24, 42, 74, 93	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	165	MET	3.1
1	A	419	GLY	2.4
1	A	163	LEU	2.2
1	A	187	ASP	2.2
1	A	409	PHE	2.2
1	A	161	GLU	2.1
1	A	234	PHE	2.1
1	A	410	PHE	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.