



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:53 AM GMT

PDB ID : 4O2W
Title : Crystal structure of the third RCC1-like domain of HERC1
Authors : Dong, A.; Hu, J.; Li, Y.; Walker, J.R.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.M.; Tong, Y.; Structural Genomics Consortium (SGC)
Deposited on : 2013-12-17
Resolution : 2.00 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>

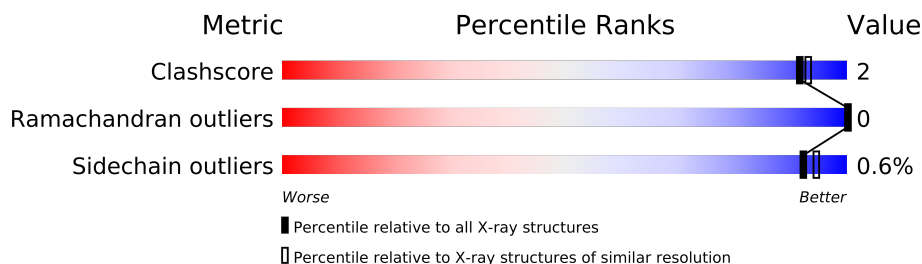
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **FAILED**
Percentile statistics : 21963
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 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	404	
1	B	404	
1	C	404	
1	D	404	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11463 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 E3 ubiquitin-protein ligase HERC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	9	0
			2725	1689	493	529	14			
1	B	365	Total	C	N	O	S	0	6	0
			2692	1669	489	519	15			
1	C	365	Total	C	N	O	S	0	3	0
			2663	1655	480	514	14			
1	D	364	Total	C	N	O	S	0	3	0
			2672	1657	481	520	14			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3957	MET	-	EXPRESSION TAG	UNP Q15751
A	3958	HIS	-	EXPRESSION TAG	UNP Q15751
A	3959	HIS	-	EXPRESSION TAG	UNP Q15751
A	3960	HIS	-	EXPRESSION TAG	UNP Q15751
A	3961	HIS	-	EXPRESSION TAG	UNP Q15751
A	3962	HIS	-	EXPRESSION TAG	UNP Q15751
A	3963	HIS	-	EXPRESSION TAG	UNP Q15751
A	3964	SER	-	EXPRESSION TAG	UNP Q15751
A	3965	SER	-	EXPRESSION TAG	UNP Q15751
A	3966	GLY	-	EXPRESSION TAG	UNP Q15751
A	3967	ARG	-	EXPRESSION TAG	UNP Q15751
A	3968	GLU	-	EXPRESSION TAG	UNP Q15751
A	3969	ASN	-	EXPRESSION TAG	UNP Q15751
A	3970	LEU	-	EXPRESSION TAG	UNP Q15751
A	3971	TYR	-	EXPRESSION TAG	UNP Q15751
A	3972	PHE	-	EXPRESSION TAG	UNP Q15751
A	3973	GLN	-	EXPRESSION TAG	UNP Q15751
A	3974	GLY	-	EXPRESSION TAG	UNP Q15751
B	3957	MET	-	EXPRESSION TAG	UNP Q15751
B	3958	HIS	-	EXPRESSION TAG	UNP Q15751
B	3959	HIS	-	EXPRESSION TAG	UNP Q15751

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3960	HIS	-	EXPRESSION TAG	UNP Q15751
B	3961	HIS	-	EXPRESSION TAG	UNP Q15751
B	3962	HIS	-	EXPRESSION TAG	UNP Q15751
B	3963	HIS	-	EXPRESSION TAG	UNP Q15751
B	3964	SER	-	EXPRESSION TAG	UNP Q15751
B	3965	SER	-	EXPRESSION TAG	UNP Q15751
B	3966	GLY	-	EXPRESSION TAG	UNP Q15751
B	3967	ARG	-	EXPRESSION TAG	UNP Q15751
B	3968	GLU	-	EXPRESSION TAG	UNP Q15751
B	3969	ASN	-	EXPRESSION TAG	UNP Q15751
B	3970	LEU	-	EXPRESSION TAG	UNP Q15751
B	3971	TYR	-	EXPRESSION TAG	UNP Q15751
B	3972	PHE	-	EXPRESSION TAG	UNP Q15751
B	3973	GLN	-	EXPRESSION TAG	UNP Q15751
B	3974	GLY	-	EXPRESSION TAG	UNP Q15751
C	3957	MET	-	EXPRESSION TAG	UNP Q15751
C	3958	HIS	-	EXPRESSION TAG	UNP Q15751
C	3959	HIS	-	EXPRESSION TAG	UNP Q15751
C	3960	HIS	-	EXPRESSION TAG	UNP Q15751
C	3961	HIS	-	EXPRESSION TAG	UNP Q15751
C	3962	HIS	-	EXPRESSION TAG	UNP Q15751
C	3963	HIS	-	EXPRESSION TAG	UNP Q15751
C	3964	SER	-	EXPRESSION TAG	UNP Q15751
C	3965	SER	-	EXPRESSION TAG	UNP Q15751
C	3966	GLY	-	EXPRESSION TAG	UNP Q15751
C	3967	ARG	-	EXPRESSION TAG	UNP Q15751
C	3968	GLU	-	EXPRESSION TAG	UNP Q15751
C	3969	ASN	-	EXPRESSION TAG	UNP Q15751
C	3970	LEU	-	EXPRESSION TAG	UNP Q15751
C	3971	TYR	-	EXPRESSION TAG	UNP Q15751
C	3972	PHE	-	EXPRESSION TAG	UNP Q15751
C	3973	GLN	-	EXPRESSION TAG	UNP Q15751
C	3974	GLY	-	EXPRESSION TAG	UNP Q15751
D	3957	MET	-	EXPRESSION TAG	UNP Q15751
D	3958	HIS	-	EXPRESSION TAG	UNP Q15751
D	3959	HIS	-	EXPRESSION TAG	UNP Q15751
D	3960	HIS	-	EXPRESSION TAG	UNP Q15751
D	3961	HIS	-	EXPRESSION TAG	UNP Q15751
D	3962	HIS	-	EXPRESSION TAG	UNP Q15751
D	3963	HIS	-	EXPRESSION TAG	UNP Q15751
D	3964	SER	-	EXPRESSION TAG	UNP Q15751
D	3965	SER	-	EXPRESSION TAG	UNP Q15751

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Chain	Residue	Modelled	Actual	Comment	Reference
D	3966	GLY	-	EXPRESSION TAG	UNP Q15751
D	3967	ARG	-	EXPRESSION TAG	UNP Q15751
D	3968	GLU	-	EXPRESSION TAG	UNP Q15751
D	3969	ASN	-	EXPRESSION TAG	UNP Q15751
D	3970	LEU	-	EXPRESSION TAG	UNP Q15751
D	3971	TYR	-	EXPRESSION TAG	UNP Q15751
D	3972	PHE	-	EXPRESSION TAG	UNP Q15751
D	3973	GLN	-	EXPRESSION TAG	UNP Q15751
D	3974	GLY	-	EXPRESSION TAG	UNP Q15751

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Cl	0	0
			3	3		
3	D	2	Total	Cl	0	0
			2	2		

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	9	Total	X	0	0
			9	9		
4	A	5	Total	X	0	0
			5	5		
4	D	8	Total	X	0	0
			8	8		
4	C	3	Total	X	0	0
			3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	194	Total 196	O 196	0	2
5	B	173	Total 174	O 174	0	1
5	C	130	Total 130	O 130	0	0
5	D	176	Total 178	O 178	0	2

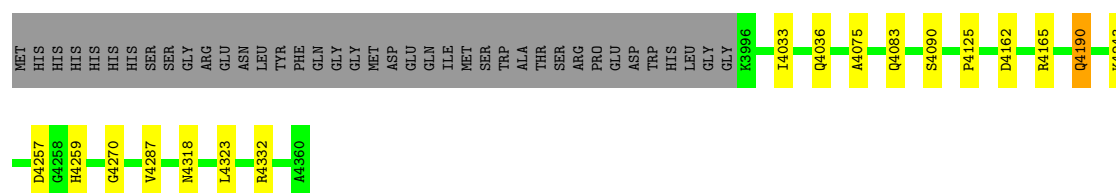
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS failed to run properly.

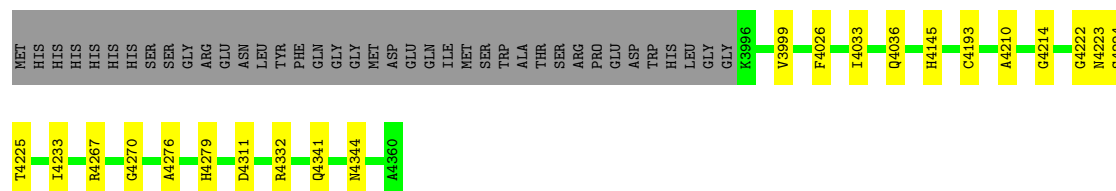
- Molecule 1: E3 ubiquitin-protein ligase HERC1

Chain A: 



- Molecule 1: E3 ubiquitin-protein ligase HERC1

Chain B: 



A4210
D4213
K4232
I4233
G4270
R4281
E4294
S4308
R4332
S4355
A4360

4 Data and refinement statistics i

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.38Å 70.90Å 105.55Å 70.93° 81.26° 90.84°	Depositor
Resolution (Å)	50.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.6 (50.00-2.00)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049, COOT 0.7.1	Depositor
R, R_{free}	0.181 , 0.221	Depositor
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.406	Xtriage
Estimated twinning fraction	0.096 for -h,k,k-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 97126 reflections	Xtriage
Total number of atoms	11463	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, MG, CL

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	0.48	0/2789	0.64	0/3774
1	B	0.50	0/2758	0.68	0/3732
1	C	0.44	0/2717	0.64	0/3683
1	D	0.49	0/2729	0.67	1/3696 (0.0%)
All	All	0.48	0/10993	0.65	1/14885 (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	D	4121	ARG	NE-CZ-NH2	-5.59	117.51	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2725	0	2642	10	0
1	B	2692	0	2622	12	0
1	C	2663	0	2560	8	0
1	D	2672	0	2586	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	3	0	0	0	0
3	D	2	0	0	0	0
4	A	5	0	0	0	0
4	B	9	0	0	0	0
4	C	3	0	0	0	0
4	D	8	0	0	0	0
5	A	196	0	0	2	0
5	B	174	0	0	2	0
5	C	130	0	0	1	0
5	D	178	0	0	1	0
All	All	11463	0	10410	41	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 2.

All (41) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4083:GLN:HG3	5:A:4641:HOH:O	1.88	0.74
1:C:4311:ASP:OD1	1:C:4341:GLN:NE2	2.22	0.73
1:B:4223:ASN:OD1	1:B:4225:THR:HG22	1.98	0.64
1:D:4083:GLN:HE21	1:D:4097:LEU:HD23	1.64	0.60
1:A:4287[A]:VAL:HG22	5:A:4529:HOH:O	2.05	0.57
1:D:4281:ARG:NE	5:D:4649:HOH:O	2.40	0.53
1:A:4190:GLN:OE1	1:A:4243:LYS:HA	2.09	0.53
1:B:4222:GLY:O	1:B:4223:ASN:HB3	2.10	0.52
1:D:4207:MET:SD	1:D:4232:LYS:NZ	2.75	0.52
1:A:4036[A]:GLN:NE2	1:A:4090:SER:O	2.43	0.52
1:B:4344:ASN:ND2	5:B:4594:HOH:O	2.42	0.51
1:B:4311:ASP:OD1	1:B:4341:GLN:NE2	2.29	0.50
1:D:4270:GLY:HA2	1:D:4332:ARG:O	2.11	0.50
1:A:4270:GLY:HA2	1:A:4332:ARG:O	2.12	0.49
1:B:4276:ALA:O	1:B:4279:HIS:HB3	2.13	0.49
1:C:4304:LEU:HD11	1:C:4355:SER:HB3	1.95	0.48
1:B:4145:HIS:CE1	1:B:4193:CYS:HB3	2.49	0.48
1:A:4075:ALA:HB3	1:A:4125:PRO:HD2	1.96	0.47
1:B:3999:VAL:HG21	1:B:4026:PHE:HB3	1.97	0.47
1:B:4270:GLY:HA2	1:B:4332:ARG:O	2.14	0.47
1:D:4210:ALA:HB2	1:D:4233:ILE:HD11	1.97	0.47
1:C:4061:GLN:HG3	1:C:4067:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:4214:GLY:O	1:B:4224:SER:HA	2.16	0.45
1:D:4099[A]:GLU:HG2	1:D:4100:SER:N	2.31	0.45
1:B:4210:ALA:HB2	1:B:4233:ILE:HD11	1.99	0.44
1:D:4294:GLU:HG3	1:D:4308:SER:HA	2.00	0.43
1:D:4196:ASN:OD1	1:D:4213:ASP:HB3	2.19	0.43
1:C:4270:GLY:HA2	1:C:4332:ARG:O	2.19	0.43
1:A:4257[A]:ASP:OD1	1:A:4259:HIS:ND1	2.52	0.42
1:D:4061:GLN:HG3	1:D:4067:LEU:HD11	2.01	0.42
1:C:4217:GLY:HA3	1:C:4280:ASN:HB3	2.00	0.42
1:D:4083:GLN:NE2	1:D:4097:LEU:HD23	2.33	0.41
1:C:4089:GLY:HA3	1:C:4143:PHE:CE2	2.54	0.41
1:A:4318:ASN:HB2	1:A:4323:LEU:HD22	2.02	0.41
1:D:4002:TRP:CE2	1:D:4355:SER:HB2	2.55	0.41
1:A:4033:ILE:HD12	1:A:4033:ILE:N	2.36	0.41
1:C:4210:ALA:HB2	1:C:4233:ILE:HD11	2.03	0.41
1:A:4162:ASP:HB2	1:A:4165:ARG:NH2	2.36	0.41
1:B:4033:ILE:HD12	1:B:4033:ILE:N	2.36	0.41
1:B:4332:ARG:NH1	5:B:4611:HOH:O	2.54	0.40
1:C:4287[B]:VAL:HG23	5:C:4527:HOH:O	2.20	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	372/404 (92%)	362 (97%)	10 (3%)	0	100	100
1	B	369/404 (91%)	361 (98%)	8 (2%)	0	100	100
1	C	366/404 (91%)	356 (97%)	10 (3%)	0	100	100
1	D	365/404 (90%)	353 (97%)	12 (3%)	0	100	100
All	All	1472/1616 (91%)	1432 (97%)	40 (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	283/312 (91%)	282 (100%)	1 (0%)	95	97
1	B	278/312 (89%)	276 (99%)	2 (1%)	91	93
1	C	269/312 (86%)	267 (99%)	2 (1%)	91	93
1	D	275/312 (88%)	274 (100%)	1 (0%)	95	97
All	All	1105/1248 (88%)	1099 (100%)	6 (0%)	92	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4190	GLN
1	B	4036	GLN
1	B	4267	ARG
1	C	4036	GLN
1	C	4190	GLN
1	D	3997	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4043	GLN
1	D	4083	GLN

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 ⓘ

Of 33 ligands modelled in this entry, 25 are unknown and 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.