



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:25 PM GMT

PDB ID : 3HO3
Title : Crystal structure of Hedgehog-interacting protein (HHIP)
Authors : Bosanac, I.; Hymowitz, S.G.
Deposited on : 2009-06-01
Resolution : 2.90 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>

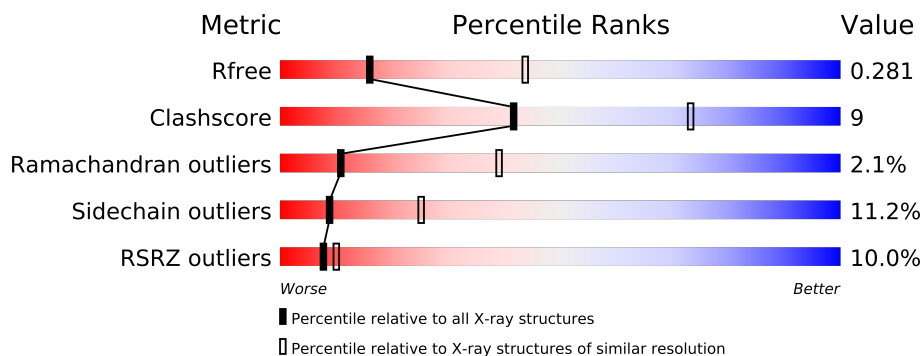
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	481	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3451 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 Hedgehog-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3451	2166	615	643	27	34	0	0

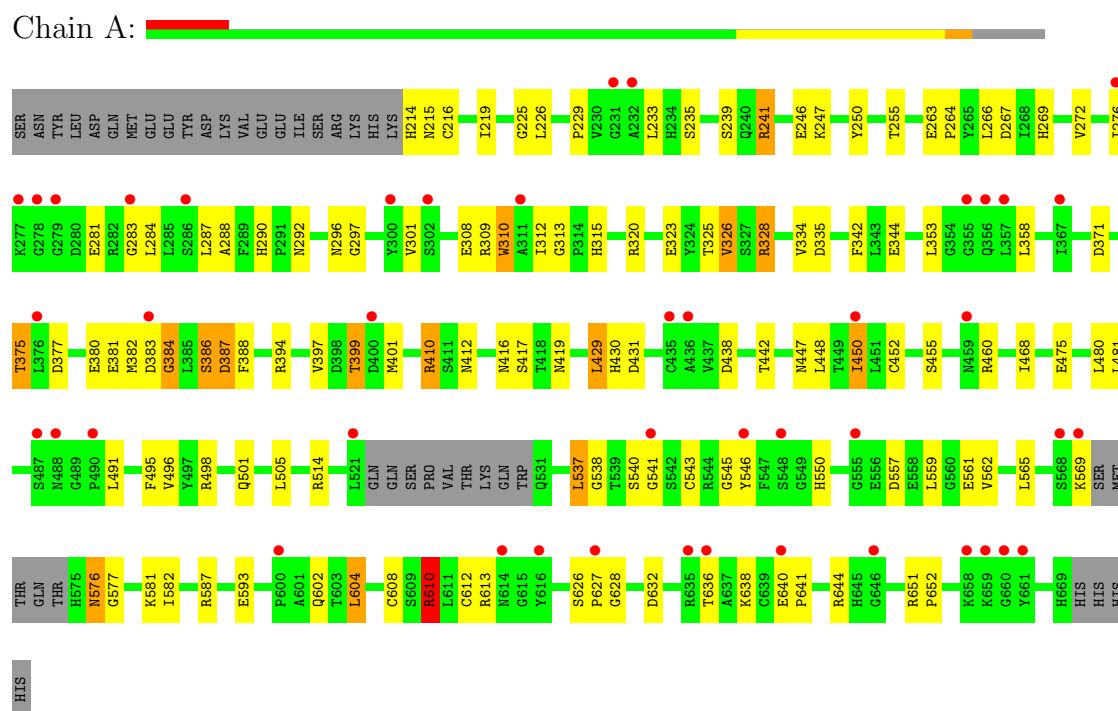
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	HIS	-	EXPRESSION TAG	UNP Q96QV1
A	669	HIS	-	EXPRESSION TAG	UNP Q96QV1
A	670	HIS	-	EXPRESSION TAG	UNP Q96QV1
A	671	HIS	-	EXPRESSION TAG	UNP Q96QV1
A	672	HIS	-	EXPRESSION TAG	UNP Q96QV1
A	673	HIS	-	EXPRESSION TAG	UNP Q96QV1

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.

- Molecule 1: Hedgehog-interacting protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	86.23Å 118.01Å 126.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.13 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.90) 96.8 (30.13-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.292 0.233 , 0.281	Depositor DCC
R_{free} test set	736 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	85.2	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 14735 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3451	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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	0.46	3/3532 (0.1%)	0.68	4/4770 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	LYS	CA-CB	13.43	1.83	1.53
1	A	638	LYS	CA-CB	-6.99	1.38	1.53
1	A	613	ARG	CA-CB	-6.66	1.39	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	LYS	CB-CA-C	-15.66	79.08	110.40
1	A	460	ARG	N-CA-CB	-13.75	85.86	110.60
1	A	460	ARG	CA-CB-CG	-7.22	97.51	113.40
1	A	569	LYS	CA-CB-CG	-6.07	100.04	113.40

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	3451	0	3351	61	0
All	All	3451	0	3351	61	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 9.

All (61) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:394:ARG:HE	1:A:412:ASN:HD21	1.15	0.91
1:A:394:ARG:HE	1:A:412:ASN:ND2	1.73	0.85
1:A:438:ASP:OD1	1:A:498:ARG:NH1	2.17	0.76
1:A:229:PRO:HB2	1:A:565:LEU:HD23	1.66	0.76
1:A:328:ARG:HH11	1:A:610:ARG:H	1.36	0.73
1:A:310:TRP:HB3	1:A:312:ILE:HG13	1.74	0.70
1:A:290:HIS:HD2	1:A:292:ASN:H	1.42	0.68
1:A:410:ARG:HD3	1:A:410:ARG:H	1.59	0.67
1:A:310:TRP:HD1	1:A:312:ILE:HD11	1.61	0.65
1:A:226:LEU:H	1:A:577:GLY:H	1.44	0.65
1:A:246:GLU:HB2	1:A:250:TYR:HB2	1.81	0.62
1:A:429:LEU:HD13	1:A:480:LEU:HD21	1.81	0.62
1:A:557:ASP:HB3	1:A:559:LEU:H	1.63	0.62
1:A:290:HIS:CD2	1:A:292:ASN:H	2.18	0.61
1:A:628:GLY:HA3	1:A:652:PRO:HB3	1.84	0.60
1:A:313:GLY:O	1:A:315:HIS:HD2	1.87	0.57
1:A:448:LEU:HD12	1:A:468:ILE:HD13	1.86	0.57
1:A:399:THR:HG22	1:A:401:MET:H	1.71	0.55
1:A:604:LEU:H	1:A:604:LEU:HD12	1.72	0.55
1:A:495:PHE:CE2	1:A:562:VAL:HG11	2.44	0.53
1:A:375:THR:HG23	1:A:377:ASP:O	2.09	0.52
1:A:328:ARG:NH1	1:A:610:ARG:H	2.06	0.52
1:A:216:CYS:HB3	1:A:538:GLY:H	1.76	0.50
1:A:342:PHE:HE1	1:A:397:VAL:HG13	1.76	0.50
1:A:281:GLU:HB3	1:A:353:LEU:CD1	2.42	0.50
1:A:229:PRO:HB2	1:A:565:LEU:CD2	2.40	0.49
1:A:386:SER:C	1:A:388:PHE:H	2.16	0.49
1:A:216:CYS:CB	1:A:538:GLY:H	2.25	0.49
1:A:537:LEU:O	1:A:545:GLY:HA3	2.13	0.48
1:A:290:HIS:CD2	1:A:296:ASN:HD21	2.31	0.48
1:A:371:ASP:HB2	1:A:430:HIS:HA	1.96	0.47
1:A:247:LYS:HG2	1:A:283:GLY:HA3	1.96	0.47
1:A:651:ARG:HB3	1:A:652:PRO:HD2	1.96	0.47
1:A:320:ARG:HG3	1:A:344:GLU:HG3	1.97	0.47
1:A:394:ARG:NE	1:A:412:ASN:HD21	1.98	0.45
1:A:640:GLU:N	1:A:641:PRO:HD2	2.32	0.45
1:A:495:PHE:CZ	1:A:562:VAL:HG11	2.52	0.45
1:A:431:ASP:HB3	1:A:455:SER:HB2	1.99	0.45
1:A:429:LEU:HD13	1:A:480:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:640:GLU:N	1:A:641:PRO:CD	2.80	0.44
1:A:383:ASP:O	1:A:384:GLY:O	2.36	0.44
1:A:239:SER:HB2	1:A:241:ARG:HD3	1.98	0.44
1:A:287:LEU:HD23	1:A:288:ALA:N	2.33	0.44
1:A:450:ILE:HD11	1:A:452:CYS:SG	2.58	0.43
1:A:219:ILE:HD11	1:A:546:TYR:O	2.19	0.43
1:A:310:TRP:CD1	1:A:312:ILE:HD11	2.47	0.43
1:A:226:LEU:N	1:A:577:GLY:H	2.12	0.43
1:A:581:LYS:HG2	1:A:582:ILE:N	2.33	0.43
1:A:501:GLN:O	1:A:587:ARG:HD3	2.19	0.43
1:A:608:CYS:O	1:A:612:CYS:HB3	2.19	0.42
1:A:284:LEU:HD11	1:A:301:VAL:HG13	2.01	0.42
1:A:263:GLU:HA	1:A:264:PRO:HD3	1.93	0.42
1:A:267:ASP:OD1	1:A:269:HIS:HB2	2.19	0.42
1:A:326:VAL:HG23	1:A:604:LEU:HD11	2.02	0.41
1:A:297:GLY:O	1:A:325:THR:HA	2.20	0.41
1:A:225:GLY:HA2	1:A:576:ASN:HA	2.03	0.41
1:A:538:GLY:C	1:A:540:SER:H	2.24	0.41
1:A:410:ARG:H	1:A:410:ARG:CD	2.22	0.41
1:A:326:VAL:HA	1:A:334:VAL:HA	2.03	0.41
1:A:214:HIS:CD2	1:A:215:ASN:H	2.39	0.40
1:A:380:GLU:C	1:A:382:MET:H	2.25	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	436/481 (91%)	396 (91%)	31 (7%)	9 (2%)	11 39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	GLY

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Mol	Chain	Res	Type
1	A	576	ASN
1	A	610	ARG
1	A	417	SER
1	A	386	SER
1	A	387	ASP
1	A	381	GLU
1	A	276	ILE
1	A	541	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	383/422 (91%)	340 (89%)	43 (11%)	9 25

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	LEU
1	A	235	SER
1	A	241	ARG
1	A	255	THR
1	A	266	LEU
1	A	272	VAL
1	A	308	GLU
1	A	309	ARG
1	A	310	TRP
1	A	323	GLU
1	A	326	VAL
1	A	328	ARG
1	A	335	ASP
1	A	358	LEU
1	A	375	THR
1	A	387	ASP
1	A	399	THR
1	A	410	ARG
1	A	416	ASN
1	A	419	ASN

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Mol	Chain	Res	Type
1	A	429	LEU
1	A	442	THR
1	A	447	ASN
1	A	450	ILE
1	A	475	GLU
1	A	481	LEU
1	A	491	LEU
1	A	496	VAL
1	A	505	LEU
1	A	514	ARG
1	A	537	LEU
1	A	543	CYS
1	A	550	HIS
1	A	561	GLU
1	A	593	GLU
1	A	602	GLN
1	A	604	LEU
1	A	610	ARG
1	A	626	SER
1	A	627	PRO
1	A	632	ASP
1	A	636	THR
1	A	644	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	A	234	HIS
1	A	290	HIS
1	A	315	HIS
1	A	403	ASN
1	A	412	ASN
1	A	414	HIS
1	A	416	ASN
1	A	459	ASN
1	A	515	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	442/481 (91%)	0.66	44 (9%) 8 10	72, 93, 122, 139	7 (1%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	546	TYR	7.0
1	A	278	GLY	4.6
1	A	488	ASN	4.5
1	A	568	SER	4.3
1	A	277	LYS	4.0
1	A	661	TYR	4.0
1	A	660	GLY	4.0
1	A	356	GLN	3.9
1	A	487	SER	3.6
1	A	276	ILE	3.6
1	A	659	LYS	3.5
1	A	383	ASP	3.4
1	A	640	GLU	3.4
1	A	302	SER	3.3
1	A	355	GLY	3.3
1	A	279	GLY	3.3
1	A	658	LYS	3.3
1	A	435	CYS	3.2
1	A	635	ARG	3.0
1	A	286	SER	2.9
1	A	231	GLY	2.9
1	A	646	GLY	2.9
1	A	548	SER	2.8
1	A	232	ALA	2.7
1	A	614	ASN	2.6
1	A	555	GLY	2.6
1	A	450	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	459	ASN	2.5
1	A	636	THR	2.5
1	A	541	GLY	2.5
1	A	357	LEU	2.5
1	A	400	ASP	2.5
1	A	436	ALA	2.4
1	A	616	TYR	2.4
1	A	569	LYS	2.4
1	A	376	LEU	2.4
1	A	627	PRO	2.3
1	A	283	GLY	2.2
1	A	490	PRO	2.1
1	A	521	LEU	2.1
1	A	311	ALA	2.1
1	A	600	PRO	2.1
1	A	300	TYR	2.0
1	A	367	ILE	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.