Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 08:38 PM EDT

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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)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
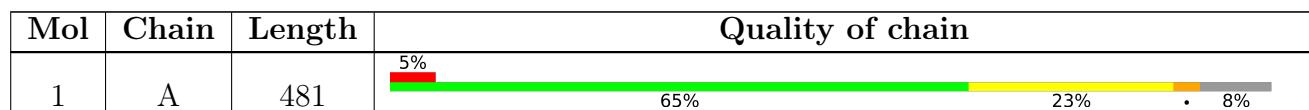
The reported resolution of this entry is 2.90 Å.

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	Percentile Ranks	Value
Rfree		0.282
Clashscore		9
Ramachandran outliers		2.1%
Sidechain outliers		11.2%
RSRZ outliers		5.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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 <=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	481	5% ■ / 65% green / 23% / · / 8%

2 Entry composition ⓘ

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total 3451	C 2166	N 615	O 643	S 27	34	0	0
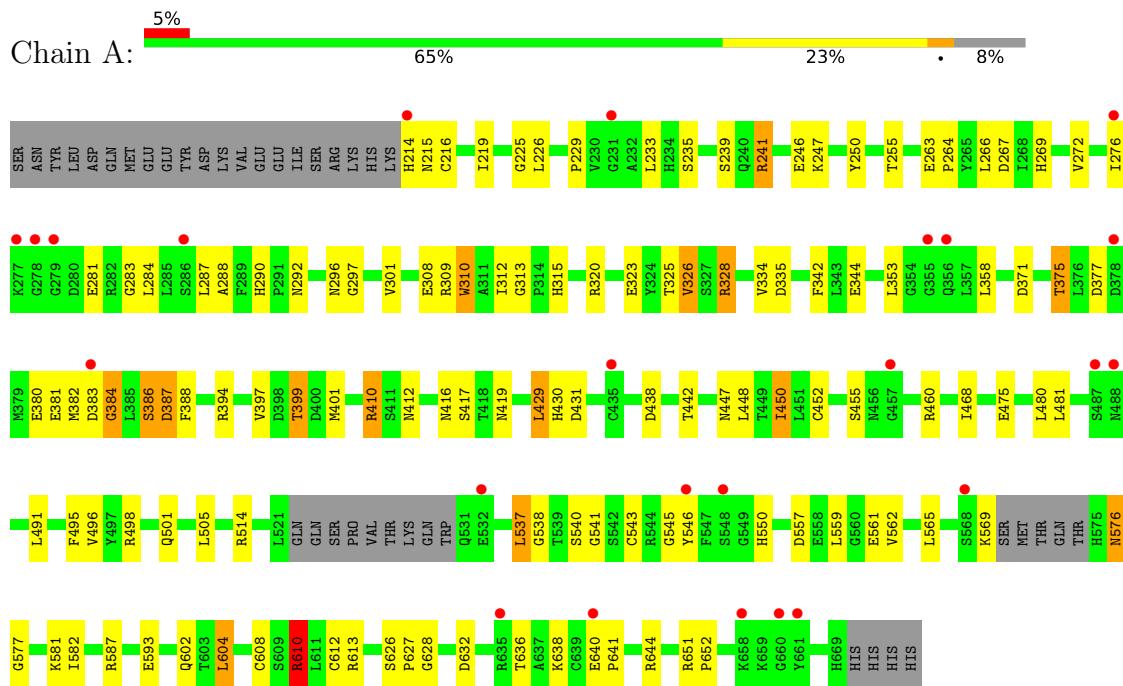
There are 6 discrepancies between the modelled and reference sequences:

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, 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: 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
$< I/\sigma(I) >$ [1]	3.86 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.292 0.232 , 0.282	Depositor DCC
R_{free} test set	736 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	85.2	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 80.2	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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	0.46	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 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	3451	0	3351	61	0
All	All	3451	0	3351	61	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 (61) 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: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:HD12	1:A:604:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:297:GLY:O	1:A:325:THR:HA	2.20	0.41
1:A:326:VAL:HG23	1:A:604:LEU:HD11	2.02	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%)	7	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	GLY
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%)	6	18

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

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Mol	Chain	Res	Type
1	A	399	THR
1	A	410	ARG
1	A	416	ASN
1	A	419	ASN
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

Sometimes 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 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 monosaccharides 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%)	0.26	24 (5%)	25	22	72, 93, 122, 139	7 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	4.7
1	A	546	TYR	4.0
1	A	383	ASP	4.0
1	A	278	GLY	3.9
1	A	661	TYR	3.8
1	A	488	ASN	3.4
1	A	568	SER	3.3
1	A	487	SER	3.3
1	A	660	GLY	3.1
1	A	548	SER	2.9
1	A	635	ARG	2.7
1	A	277	LYS	2.6
1	A	355	GLY	2.5
1	A	356	GLN	2.5
1	A	457	GLY	2.4
1	A	532	GLU	2.3
1	A	276	ILE	2.2
1	A	658	LYS	2.2
1	A	640	GLU	2.2
1	A	214	HIS	2.1
1	A	231	GLY	2.1
1	A	286	SER	2.1
1	A	378	ASP	2.0
1	A	435	CYS	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 monosaccharides 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.