



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:58 AM UTC

PDB ID : 3D1M / pdb_00003d1m
Title : Crystal Structure of Sonic Hedgehog Bound to the third FNIII domain of CDO
Authors : McLellan, J.S.; Leahy, D.J.
Deposited on : 2008-05-06
Resolution : 1.70 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

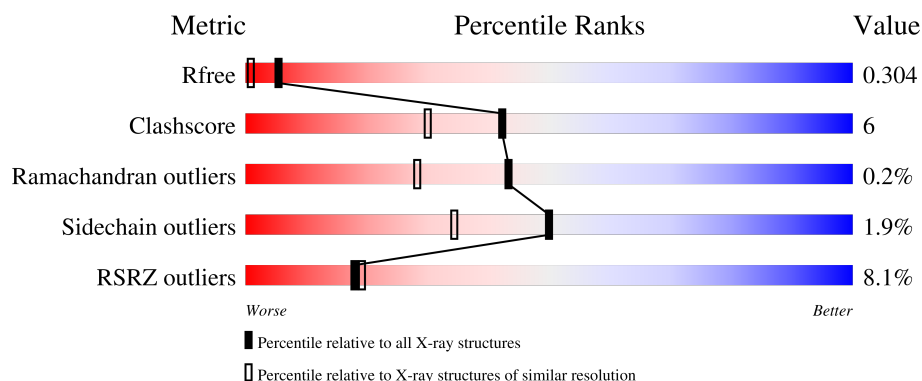
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 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 $\leq 5\%$. 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	168	7% 79% 9% 12%
1	B	168	% 79% 10% 11%
2	C	102	15% 73% 12% 15%
2	D	102	11% 81% 14% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4327 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 Sonic hedgehog protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1189	743	212	229	5			
1	B	150	Total	C	N	O	S	0	0	0
			1207	754	214	234	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q62226
A	23	PRO	-	expression tag	UNP Q62226
A	24	GLY	-	expression tag	UNP Q62226
A	25	SER	-	expression tag	UNP Q62226
B	22	GLY	-	expression tag	UNP Q62226
B	23	PRO	-	expression tag	UNP Q62226
B	24	GLY	-	expression tag	UNP Q62226
B	25	SER	-	expression tag	UNP Q62226

- Molecule 2 is a protein called Cell adhesion molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	87	Total	C	N	O	S	0	0	0
			714	450	114	144	6			
2	D	99	Total	C	N	O	S	0	0	0
			801	503	129	163	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	823	GLY	-	expression tag	UNP Q4KMG0
C	824	SER	-	expression tag	UNP Q4KMG0
C	825	THR	-	expression tag	UNP Q4KMG0
D	823	GLY	-	expression tag	UNP Q4KMG0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	824	SER	-	expression tag	UNP Q4KMG0
D	825	THR	-	expression tag	UNP Q4KMG0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	2	Total Ca 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	136	Total O 136 136	0	0
5	B	136	Total O 136 136	0	0
5	C	62	Total O 62 62	0	0
5	D	76	Total O 76 76	0	0

i

- Molecule 1: Sonic hedgehog protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.18Å 98.58Å 144.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.56 – 1.70 30.56 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.56-1.70) 99.0 (30.56-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.229 (Not available) , 0.304	Depositor DCC
R_{free} test set	2693 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4327	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN

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	0.72	0/1215	0.84	0/1640
1	B	0.75	0/1233	0.84	0/1663
2	C	0.96	3/732 (0.4%)	0.90	2/987 (0.2%)
2	D	0.79	0/823	0.89	1/1116 (0.1%)
All	All	0.79	3/4003 (0.1%)	0.86	3/5406 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	860	GLN	CD-NE2	8.31	1.50	1.33
2	C	860	GLN	CD-OE1	6.43	1.35	1.23
2	C	913	SER	C-O	6.17	1.31	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	906	CYS	N-CA-C	-5.77	101.48	110.42
2	D	867	ARG	CG-CD-NE	-5.56	99.77	112.00
2	C	884	GLY	N-CA-C	5.28	120.48	114.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1189	0	1149	11	0
1	B	1207	0	1166	14	0
2	C	714	0	655	16	0
2	D	801	0	742	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	136	0	0	2	0
5	B	136	0	0	2	0
5	C	62	0	0	0	0
5	D	76	0	0	1	0
All	All	4327	0	3712	48	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 6.

All (48) 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)
2:C:890:MET:CE	2:D:890:MET:HE3	1.92	0.99
2:C:842:GLN:HE22	2:D:842:GLN:HE22	1.14	0.93
2:C:844:MET:HE3	2:D:844:MET:HE2	1.64	0.79
1:A:134:HIS:HD2	5:D:130:HOH:O	1.67	0.76
2:C:890:MET:HE3	2:D:890:MET:HE3	1.68	0.76
2:C:844:MET:CE	2:C:890:MET:HE2	2.20	0.72
2:C:890:MET:CE	2:D:890:MET:CE	2.69	0.70
2:C:890:MET:HE1	2:D:890:MET:HE3	1.74	0.70
1:A:55:LYS:CD	5:A:251:HOH:O	2.40	0.69
2:C:844:MET:HE3	2:D:844:MET:CE	2.26	0.65
1:A:55:LYS:HD2	5:A:251:HOH:O	2.00	0.62
1:B:80:ASN:HD22	1:B:80:ASN:C	2.08	0.62
2:D:830:PRO:HG2	2:D:904:MET:HE2	1.82	0.61
1:B:80:ASN:HD21	1:B:82:ASN:HB2	1.64	0.60
1:A:63:TYR:CE1	1:A:138:GLU:HA	2.37	0.60
1:B:80:ASN:HD22	1:B:82:ASN:H	1.52	0.57
1:B:116:ASN:HB2	5:B:274:HOH:O	2.04	0.57
1:B:80:ASN:ND2	1:B:82:ASN:H	2.04	0.56
1:A:63:TYR:CZ	1:A:138:GLU:HA	2.42	0.54
2:C:862:PHE:HB2	2:C:882:VAL:HG22	1.90	0.53
2:D:862:PHE:HB2	2:D:882:VAL:HG22	1.89	0.53
1:A:137:GLU:H	1:A:137:GLU:CD	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:O	1:B:76:GLU:HG2	2.10	0.51
1:A:63:TYR:CD1	1:A:143:GLU:OE2	2.64	0.50
2:C:844:MET:CE	2:C:890:MET:CE	2.89	0.50
1:B:80:ASN:HD21	1:B:82:ASN:CB	2.25	0.49
1:B:145:ARG:HD2	1:B:186:VAL:O	2.13	0.49
2:D:909:GLU:H	2:D:909:GLU:CD	2.21	0.49
2:C:849:TYR:CE2	2:C:859:ILE:HD11	2.49	0.48
2:C:849:TYR:HE2	2:C:859:ILE:HD11	1.78	0.47
1:A:45:TYR:CZ	1:A:46:LYS:HE2	2.50	0.47
1:A:88:LYS:HE3	1:A:90:GLU:HB3	1.97	0.47
1:B:145:ARG:HD3	1:B:188:ALA:HA	1.96	0.46
2:C:844:MET:HE2	2:C:890:MET:CE	2.47	0.45
1:A:145:ARG:HD2	1:A:186:VAL:O	2.17	0.45
1:B:88:LYS:HE3	1:B:90:GLU:HB3	1.98	0.45
2:D:859:ILE:HD12	2:D:906:CYS:HB2	1.98	0.45
1:B:179:LYS:HD2	2:C:897:GLU:OE1	2.16	0.45
1:B:99:MET:HG3	1:B:104:LYS:HG3	1.99	0.44
2:D:859:ILE:HD11	2:D:862:PHE:CZ	2.53	0.44
1:B:144:GLY:HA2	5:B:308:HOH:O	2.17	0.44
2:C:844:MET:HE2	2:C:890:MET:HE2	1.98	0.43
1:B:49:ILE:HA	1:B:50:PRO:C	2.43	0.43
2:D:830:PRO:CG	2:D:904:MET:HE2	2.48	0.43
2:D:826:PRO:HD3	2:D:908:ASN:CG	2.44	0.42
1:A:49:ILE:HA	1:A:50:PRO:C	2.46	0.41
2:D:866:TYR:HA	2:D:901:ASP:O	2.20	0.41
2:C:844:MET:CE	2:D:844:MET:CE	2.97	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	146/168 (87%)	144 (99%)	2 (1%)	0	100	100
1	B	148/168 (88%)	146 (99%)	2 (1%)	0	100	100
2	C	83/102 (81%)	80 (96%)	2 (2%)	1 (1%)	10	2
2	D	97/102 (95%)	93 (96%)	4 (4%)	0	100	100
All	All	474/540 (88%)	463 (98%)	10 (2%)	1 (0%)	43	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	913	SER

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	126/140 (90%)	125 (99%)	1 (1%)	73	65
1	B	128/140 (91%)	125 (98%)	3 (2%)	44	27
2	C	79/93 (85%)	78 (99%)	1 (1%)	61	48
2	D	91/93 (98%)	88 (97%)	3 (3%)	33	17
All	All	424/466 (91%)	416 (98%)	8 (2%)	50	34

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	B	43	LEU
1	B	62	ARG
1	B	80	ASN
2	C	883	GLU
2	D	827	ILE
2	D	859	ILE
2	D	882	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	B	51	ASN
1	B	80	ASN
2	C	842	GLN
2	C	860	GLN
2	D	855	ASN
2	D	893	HIS
2	D	905	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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	148/168 (88%)	0.90	11 (7%) 20 22	29, 32, 42, 47	0
1	B	150/168 (89%)	0.50	2 (1%) 75 79	27, 30, 39, 46	0
2	C	87/102 (85%)	1.24	15 (17%) 4 3	29, 33, 44, 52	0
2	D	99/102 (97%)	1.20	11 (11%) 10 10	28, 32, 44, 49	0
All	All	484/540 (89%)	0.90	39 (8%) 18 19	27, 32, 43, 52	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	826	PRO	4.0
1	A	63	TYR	4.0
2	D	853	SER	3.7
2	D	827	ILE	3.5
2	C	829	GLY	3.4
1	A	70	ASN	3.4
2	C	911	GLY	3.4
2	D	857	THR	3.4
2	D	854	ASN	3.4
2	C	910	GLY	3.2
2	C	849	TYR	3.0
2	C	907	PHE	2.9
1	A	180	ALA	2.8
2	D	828	THR	2.7
2	C	873	ASN	2.6
2	C	875	SER	2.5
2	C	834	TYR	2.5
1	A	48	PHE	2.4
2	C	920	ILE	2.4
1	B	76	GLU	2.4
1	B	70	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	852	SER	2.3
2	C	874	ASP	2.2
1	A	74	PHE	2.2
2	D	890	MET	2.2
1	A	114	VAL	2.2
1	A	121	VAL	2.2
1	A	45	TYR	2.2
2	D	858	PRO	2.2
2	C	913	SER	2.2
1	A	75	LYS	2.1
2	D	856	ASN	2.1
2	C	859	ILE	2.1
2	D	850	ILE	2.1
1	A	53	ALA	2.1
2	C	918	VAL	2.1
2	C	908	ASN	2.1
1	A	41	THR	2.1
2	C	883	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	A	1	1/1	0.98	0.15	25,25,25,25	1
3	ZN	B	2	1/1	0.98	0.12	26,26,26,26	1
4	CA	A	190	1/1	0.99	0.14	19,19,19,19	0
4	CA	A	2	1/1	0.99	0.10	21,21,21,21	0
4	CA	B	3	1/1	0.99	0.13	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	B	4	1/1	1.00	0.10	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.