



Full wwPDB Geometry-Only Validation Report ⓘ

Mar 4, 2026 – 10:14 PM UTC

PDB ID : 2HS7 / pdb_00002hs7
Title : Multipattern rietveld refinement with protein powder data: An approach to higher resolution
Authors : Von Dreele, R.B.
Deposited on : 2006-07-21
Resolution : 1.98 Å(reported)

This is a Full wwPDB Geometry-Only 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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

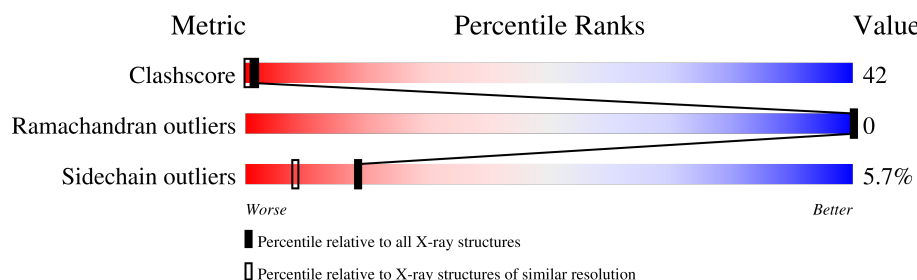
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

POWDER DIFFRACTION

The reported resolution of this entry is 1.98 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	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	129	 44% 47% 7% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1098 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 Lysozyme C.

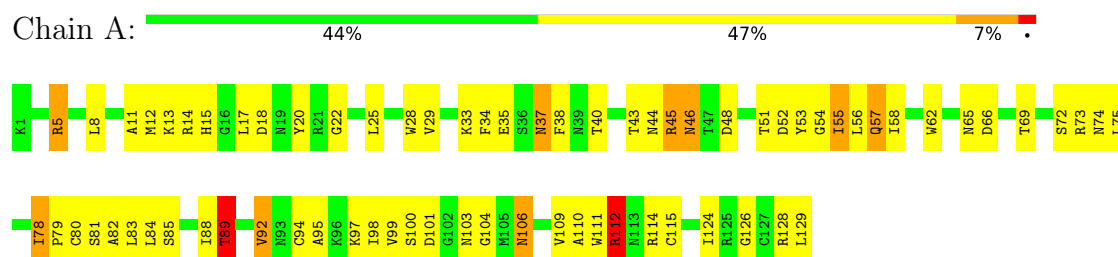
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	97	Total	O	0	0
			97	97		

Note EDS was not executed.

- Molecule 1: Lysozyme C



4 Model quality [i](#)

4.1 Standard geometry [i](#)

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	1.17	2/1021 (0.2%)	1.39	10/1379 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	ILE	CA-C	5.58	1.58	1.52
1	A	51	THR	CA-C	5.18	1.58	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ASN	CA-CB-CG	6.35	118.95	112.60
1	A	78	ILE	N-CA-C	5.77	113.92	109.19
1	A	55	ILE	CA-CB-CG1	5.71	120.10	110.40
1	A	89	THR	CA-C-N	-5.49	111.54	120.71
1	A	89	THR	C-N-CA	-5.49	111.54	120.71
1	A	106	ASN	N-CA-C	-5.43	106.63	113.20
1	A	112	ARG	CA-C-N	-5.30	113.91	122.23
1	A	112	ARG	C-N-CA	-5.30	113.91	122.23
1	A	101	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	46	ASN	CA-CB-CG	5.24	117.84	112.60

There are no chirality outliers.

There are no planarity outliers.

4.2 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	1001	0	959	83	1
2	A	97	0	0	8	1
All	All	1098	0	959	83	1

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 42.

All (83) 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:111:TRP:HA	1:A:115:CYS:HB3	1.52	0.90
1:A:112:ARG:HH11	1:A:112:ARG:CB	1.88	0.87
1:A:57:GLN:HE21	1:A:57:GLN:HA	1.44	0.83
1:A:112:ARG:HH11	1:A:112:ARG:CG	1.95	0.79
1:A:112:ARG:HH11	1:A:112:ARG:HB2	1.49	0.77
1:A:97:LYS:HA	1:A:100:SER:HB2	1.67	0.76
1:A:25:LEU:HA	1:A:28:TRP:HD1	1.50	0.76
1:A:13:LYS:HG3	1:A:18:ASP:HB2	1.68	0.75
1:A:89:THR:O	1:A:89:THR:CG2	2.37	0.72
1:A:124:ILE:O	1:A:124:ILE:HG22	1.89	0.71
1:A:62:TRP:HB2	1:A:73:ARG:HB2	1.73	0.70
1:A:12:MET:HA	1:A:15:HIS:HB2	1.77	0.67
1:A:40:THR:HA	1:A:55:ILE:HB	1.74	0.67
1:A:89:THR:O	1:A:89:THR:HG22	1.94	0.66
1:A:13:LYS:HD2	1:A:129:LEU:HD13	1.77	0.66
1:A:43:THR:HG22	1:A:53:TYR:HA	1.77	0.65
1:A:112:ARG:HG2	1:A:112:ARG:NH1	2.11	0.65
1:A:53:TYR:HD2	1:A:84:LEU:HD11	1.62	0.64
1:A:34:PHE:HB3	1:A:110:ALA:HB1	1.81	0.62
1:A:57:GLN:HA	1:A:57:GLN:NE2	2.14	0.61
1:A:81:SER:HA	1:A:84:LEU:HD12	1.84	0.60
1:A:14:ARG:HG2	1:A:14:ARG:O	2.01	0.59
1:A:112:ARG:CG	1:A:112:ARG:NH1	2.56	0.58
1:A:53:TYR:O	1:A:58:ILE:N	2.38	0.56
1:A:8:LEU:HD12	1:A:88:ILE:HD11	1.86	0.56
1:A:62:TRP:HA	1:A:73:ARG:H	1.71	0.56
1:A:5:ARG:NH2	2:A:173:HOH:O	2.38	0.56
1:A:54:GLY:H	1:A:84:LEU:HD21	1.70	0.56
1:A:128:ARG:HG3	1:A:128:ARG:HH11	1.71	0.55
1:A:45:ARG:HD2	1:A:46:ASN:O	2.06	0.55
1:A:12:MET:HE2	1:A:17:LEU:HD12	1.89	0.53
1:A:33:LYS:HG2	2:A:192:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:O	1:A:112:ARG:HB3	2.08	0.53
1:A:44:ASN:ND2	1:A:57:GLN:OE1	2.42	0.52
1:A:111:TRP:HA	1:A:115:CYS:CB	2.33	0.51
1:A:94:CYS:SG	1:A:94:CYS:O	2.68	0.51
1:A:103:ASN:HB2	2:A:135:HOH:O	2.09	0.51
1:A:25:LEU:HB3	1:A:124:ILE:HD11	1.93	0.51
1:A:38:PHE:N	1:A:38:PHE:CD1	2.79	0.49
1:A:13:LYS:HD3	1:A:129:LEU:HB3	1.95	0.49
1:A:56:LEU:HD13	1:A:95:ALA:HB2	1.93	0.48
1:A:11:ALA:HB1	1:A:15:HIS:CE1	2.48	0.48
1:A:54:GLY:HA2	1:A:83:LEU:O	2.14	0.48
1:A:11:ALA:C	1:A:15:HIS:HD1	2.21	0.48
1:A:53:TYR:OH	1:A:66:ASP:HB2	2.13	0.48
1:A:34:PHE:CD2	1:A:114:ARG:HG2	2.49	0.48
1:A:124:ILE:O	1:A:124:ILE:CG2	2.62	0.48
1:A:85:SER:HB3	2:A:201:HOH:O	2.13	0.48
1:A:5:ARG:HA	1:A:38:PHE:HE2	1.79	0.47
1:A:11:ALA:HB3	1:A:88:ILE:HD12	1.97	0.47
1:A:43:THR:HA	1:A:52:ASP:O	2.15	0.47
1:A:17:LEU:CD1	1:A:92:VAL:HG22	2.43	0.47
1:A:97:LYS:HA	1:A:100:SER:CB	2.40	0.47
1:A:94:CYS:O	1:A:98:ILE:HG13	2.14	0.47
1:A:11:ALA:CB	1:A:88:ILE:HD12	2.45	0.47
1:A:33:LYS:HA	1:A:37:ASN:HA	1.96	0.46
1:A:69:THR:HB	1:A:72:SER:HB3	1.98	0.46
1:A:25:LEU:O	1:A:29:VAL:HG23	2.16	0.45
1:A:112:ARG:HB2	1:A:112:ARG:NH1	2.26	0.45
1:A:12:MET:CE	1:A:28:TRP:HB3	2.46	0.45
1:A:14:ARG:NH1	2:A:146:HOH:O	2.49	0.45
1:A:78:ILE:HG22	1:A:79:PRO:O	2.17	0.45
1:A:11:ALA:O	1:A:15:HIS:ND1	2.42	0.45
1:A:62:TRP:CZ3	1:A:75:LEU:HD12	2.52	0.45
1:A:100:SER:HB3	2:A:203:HOH:O	2.17	0.44
1:A:34:PHE:CB	1:A:110:ALA:HB1	2.45	0.43
1:A:66:ASP:N	1:A:66:ASP:OD1	2.37	0.43
1:A:65:ASN:HB2	1:A:74:ASN:OD1	2.18	0.43
1:A:48:ASP:N	1:A:48:ASP:OD1	2.51	0.43
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.86	0.43
1:A:78:ILE:CG2	1:A:82:ALA:HB3	2.49	0.42
1:A:35:GLU:HB3	1:A:57:GLN:CG	2.50	0.42
1:A:12:MET:HE2	1:A:17:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:C	1:A:106:ASN:H	2.28	0.42
1:A:25:LEU:HA	1:A:28:TRP:CD1	2.41	0.41
1:A:8:LEU:HD12	1:A:88:ILE:CD1	2.50	0.41
1:A:40:THR:O	1:A:84:LEU:HD23	2.20	0.41
1:A:17:LEU:HD11	1:A:92:VAL:HG22	2.03	0.41
1:A:53:TYR:CD2	1:A:80:CYS:HB3	2.56	0.41
1:A:20:TYR:HE2	1:A:99:VAL:HG23	1.86	0.41
1:A:126:GLY:HA3	2:A:165:HOH:O	2.21	0.41
1:A:40:THR:HG22	2:A:219:HOH:O	2.20	0.41
1:A:112:ARG:HH11	1:A:112:ARG:HG2	1.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLY:O	2:A:189:HOH:O[4_455]	2.10	0.10

4.3 Torsion angles [i](#)

4.3.1 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	127/129 (98%)	124 (98%)	3 (2%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 Protein sidechains [i](#)

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	105/105 (100%)	99 (94%)	6 (6%)	18 8

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

Mol	Chain	Res	Type
1	A	5	ARG
1	A	45	ARG
1	A	57	GLN
1	A	89	THR
1	A	92	VAL
1	A	112	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	44	ASN
1	A	57	GLN
1	A	113	ASN

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

4.6 Ligand geometry ⓘ

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.