



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:33 PM UTC

PDB ID : 5H7B / pdb_00005h7b
Title : Crystal structure of a repeat protein with five Protein A repeat modules
Authors : Youn, S.J.; Kwon, N.Y.; Lee, J.H.; Kim, J.H.; Lee, H.; Lee, J.O.
Deposited on : 2016-11-17
Resolution : 3.10 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

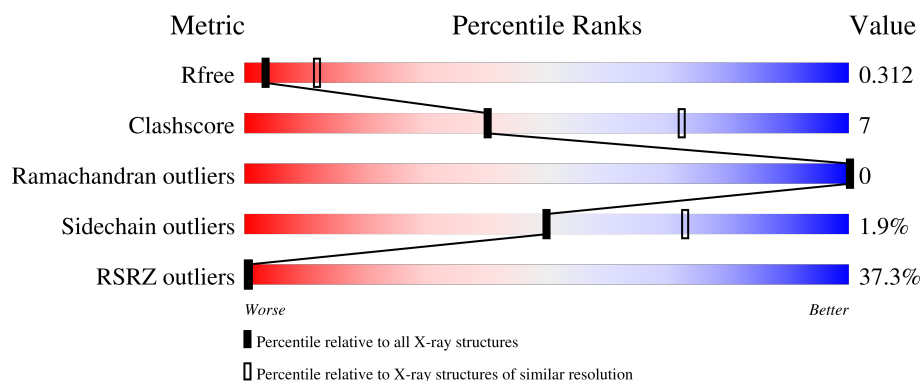
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	237	16% 83% 13% ..
1	B	237	50% 63% 17% 19%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3387 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 Immunoglobulin G-binding protein A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	0	0	0
			1845	1149	321	375			
1	B	191	Total	C	N	O	0	0	0
			1542	964	266	312			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	expression tag	UNP P38507
A	31	SER	-	expression tag	UNP P38507
A	32	HIS	-	expression tag	UNP P38507
A	33	MET	-	expression tag	UNP P38507
A	59	ALA	GLY	engineered mutation	UNP P38507
A	86	ALA	ASN	engineered mutation	UNP P38507
A	93	SER	HIS	engineered mutation	UNP P38507
A	104	ALA	GLY	engineered mutation	UNP P38507
A	131	ALA	ASN	engineered mutation	UNP P38507
A	149	ALA	GLY	engineered mutation	UNP P38507
A	176	ALA	ASN	engineered mutation	UNP P38507
A	194	ALA	GLY	engineered mutation	UNP P38507
A	221	ALA	ASN	engineered mutation	UNP P38507
A	239	ALA	GLY	engineered mutation	UNP P38507
B	30	GLY	-	expression tag	UNP P38507
B	31	SER	-	expression tag	UNP P38507
B	32	HIS	-	expression tag	UNP P38507
B	33	MET	-	expression tag	UNP P38507
B	59	ALA	GLY	engineered mutation	UNP P38507
B	86	ALA	ASN	engineered mutation	UNP P38507
B	93	SER	HIS	engineered mutation	UNP P38507
B	104	ALA	GLY	engineered mutation	UNP P38507
B	131	ALA	ASN	engineered mutation	UNP P38507
B	149	ALA	GLY	engineered mutation	UNP P38507
B	176	ALA	ASN	engineered mutation	UNP P38507

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Chain	Residue	Modelled	Actual	Comment	Reference
B	194	ALA	GLY	engineered mutation	UNP P38507
B	221	ALA	ASN	engineered mutation	UNP P38507
B	239	ALA	GLY	engineered mutation	UNP P38507

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.89Å 45.64Å 82.14Å 90.00° 105.72° 90.00°	Depositor
Resolution (Å)	39.53 – 3.10 39.53 – 3.10	Depositor EDS
% Data completeness (in resolution range)	74.5 (39.53-3.10) 76.7 (39.53-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.56 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.269 , 0.315 0.271 , 0.312	Depositor DCC
R_{free} test set	420 reflections (3.78%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 91.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	3387	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% 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](#)

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	0.15	0/1873	0.46	0/2532
1	B	0.13	0/1567	0.34	0/2119
All	All	0.14	0/3440	0.41	0/4651

There are no bond length outliers.

There are no bond angle outliers.

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	1845	0	1793	18	0
1	B	1542	0	1491	26	0
All	All	3387	0	3284	44	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 7.

All (44) 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:186:ASN:O	1:A:220:GLN:NE2	2.13	0.80
1:B:130:GLN:O	1:B:133:PHE:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE2	1:A:192:ARG:NH1	2.27	0.66
1:A:39:GLN:O	1:A:43:PHE:HB2	1.96	0.65
1:A:227:LEU:HD21	1:A:241:ILE:HD11	1.79	0.65
1:B:148:ASN:O	1:B:152:GLN:HB2	1.97	0.64
1:A:152:GLN:NE2	1:A:156:ASP:OD1	2.33	0.61
1:B:109:LEU:HD21	1:B:116:SER:HA	1.83	0.60
1:A:229:LEU:O	1:A:237:ARG:NH2	2.36	0.59
1:A:158:PRO:O	1:A:161:SER:OG	2.21	0.57
1:A:139:LEU:O	1:A:147:ARG:NH2	2.37	0.56
1:B:139:LEU:O	1:B:147:ARG:NH2	2.32	0.56
1:A:212:GLU:HA	1:A:215:LYS:HE3	1.87	0.56
1:A:214:LYS:O	1:A:217:ASN:HB3	2.08	0.53
1:B:99:GLU:O	1:B:103:ASN:ND2	2.44	0.51
1:B:88:PHE:HE1	1:B:109:LEU:HD22	1.75	0.50
1:B:223:PHE:O	1:B:227:LEU:HB2	2.12	0.50
1:A:122:GLU:HA	1:A:125:LYS:HE3	1.95	0.48
1:A:109:LEU:HD21	1:A:116:SER:HA	1.97	0.46
1:B:109:LEU:HG	1:B:119:LEU:HD13	1.97	0.46
1:B:175:GLN:O	1:B:178:PHE:HB2	2.16	0.46
1:B:95:PRO:HA	1:B:102:ARG:HH21	1.81	0.46
1:B:68:PRO:O	1:B:71:SER:OG	2.25	0.45
1:B:210:LEU:HG	1:B:214:LYS:HE2	1.99	0.44
1:B:178:PHE:O	1:B:182:LEU:HB2	2.17	0.44
1:A:100:GLU:O	1:A:104:ALA:HB2	2.17	0.44
1:B:148:ASN:O	1:B:152:GLN:CB	2.62	0.44
1:B:88:PHE:CD1	1:B:109:LEU:HD13	2.53	0.44
1:B:94:LEU:HB3	1:B:127:ASN:OD1	2.18	0.43
1:B:158:PRO:HA	1:B:161:SER:HB3	2.00	0.43
1:B:92:LEU:HD13	1:B:106:ILE:HD11	2.00	0.43
1:B:165:LEU:O	1:B:168:ALA:HB3	2.19	0.43
1:A:229:LEU:HA	1:A:229:LEU:HD12	1.71	0.42
1:B:181:ILE:O	1:B:192:ARG:HD3	2.20	0.42
1:B:190:GLU:O	1:B:194:ALA:HB2	2.20	0.41
1:B:43:PHE:CD1	1:B:61:ILE:HD12	2.56	0.41
1:A:109:LEU:HD21	1:A:116:SER:CA	2.50	0.41
1:A:181:ILE:HA	1:A:184:LEU:HG	2.03	0.41
1:B:86:ALA:O	1:B:89:TYR:HB3	2.21	0.41
1:A:178:PHE:O	1:A:182:LEU:HB2	2.21	0.41
1:B:85:GLN:HA	1:B:88:PHE:CD2	2.56	0.41
1:B:49:LEU:O	1:B:57:ARG:NH1	2.54	0.41
1:B:139:LEU:HD23	1:B:139:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:PHE:HD1	1:A:240:PHE:HA	1.76	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	228/237 (96%)	217 (95%)	11 (5%)	0	100	100
1	B	189/237 (80%)	175 (93%)	14 (7%)	0	100	100
All	All	417/474 (88%)	392 (94%)	25 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 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	199/205 (97%)	193 (97%)	6 (3%)	36	65
1	B	166/205 (81%)	165 (99%)	1 (1%)	78	83
All	All	365/410 (89%)	358 (98%)	7 (2%)	50	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	109	LEU
1	A	145	GLU
1	A	199	LEU
1	A	229	LEU
1	A	240	PHE
1	B	109	LEU

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	191	GLN
1	A	220	GLN
1	A	236	GLN
1	A	265	GLN
1	B	138	HIS
1	B	146	GLN
1	B	191	GLN
1	B	220	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](#)

There are no ligands in this entry.

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	230/237 (97%)	1.07	38 (16%) 4 2	8, 34, 81, 103	0
1	B	191/237 (80%)	2.69	119 (62%) 0 0	25, 97, 146, 186	0
All	All	421/474 (88%)	1.80	157 (37%) 1 0	8, 51, 137, 186	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	ASP	8.6
1	B	116	SER	7.6
1	B	223	PHE	6.8
1	B	123	ALA	6.6
1	B	226	ILE	6.5
1	B	222	ALA	6.3
1	B	115	GLN	5.8
1	B	179	TYR	5.6
1	B	149	ALA	5.5
1	B	88	PHE	5.3
1	B	193	ASN	5.3
1	A	206	SER	5.1
1	B	160	GLN	5.0
1	B	114	SER	5.0
1	B	185	PRO	4.9
1	B	134	TYR	4.9
1	A	99	GLU	4.9
1	B	43	PHE	4.9
1	B	183	HIS	4.9
1	B	117	ALA	4.9
1	B	139	LEU	4.7
1	B	165	LEU	4.7
1	B	38	GLU	4.7
1	B	197	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	136	ILE	4.6
1	B	199	LEU	4.6
1	B	209	LEU	4.6
1	B	98	ASN	4.4
1	B	187	LEU	4.4
1	B	227	LEU	4.4
1	B	118	ASN	4.3
1	B	184	LEU	4.2
1	B	113	PRO	4.2
1	B	150	PHE	4.2
1	B	154	LEU	4.2
1	B	221	ALA	4.2
1	A	193	ASN	4.1
1	B	151	ILE	4.1
1	A	246	ASP	4.1
1	B	212	GLU	4.0
1	B	210	LEU	4.0
1	B	45	GLU	4.0
1	B	112	ASP	3.9
1	A	108	SER	3.9
1	B	169	LYS	3.9
1	A	88	PHE	3.8
1	B	208	ASN	3.8
1	A	208	ASN	3.7
1	B	157	ASP	3.7
1	B	155	LYS	3.7
1	B	172	ASN	3.7
1	B	182	LEU	3.7
1	B	175	GLN	3.6
1	B	100	GLU	3.6
1	B	211	ALA	3.6
1	B	67	ASP	3.6
1	B	89	TYR	3.6
1	B	225	GLU	3.6
1	B	77	GLU	3.5
1	B	147	ARG	3.5
1	B	152	GLN	3.5
1	B	213	ALA	3.5
1	B	42	ALA	3.5
1	B	156	ASP	3.5
1	B	224	TYR	3.5
1	B	103	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	174	GLN	3.5
1	B	190	GLU	3.4
1	A	103	ASN	3.4
1	B	171	LEU	3.4
1	B	216	LEU	3.4
1	B	41	ASN	3.4
1	B	217	ASN	3.4
1	B	195	PHE	3.4
1	A	41	ASN	3.4
1	B	204	SER	3.4
1	B	228	HIS	3.4
1	A	118	ASN	3.3
1	B	54	GLU	3.3
1	B	144	GLU	3.3
1	B	220	GLN	3.3
1	B	181	ILE	3.3
1	B	194	ALA	3.3
1	B	218	GLU	3.3
1	A	189	GLU	3.3
1	A	252	ALA	3.2
1	B	207	ALA	3.1
1	B	198	SER	3.1
1	A	112	ASP	3.1
1	B	158	PRO	3.1
1	B	166	ALA	3.1
1	B	205	GLN	3.1
1	A	251	SER	3.1
1	B	215	LYS	3.1
1	A	83	GLU	3.0
1	B	99	GLU	3.0
1	B	161	SER	3.0
1	B	214	LYS	2.9
1	A	154	LEU	2.9
1	A	218	GLU	2.9
1	B	145	GLU	2.9
1	B	200	LYS	2.9
1	B	101	GLN	2.8
1	B	202	ASP	2.8
1	B	180	GLU	2.8
1	B	153	SER	2.8
1	B	142	LEU	2.8
1	B	146	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	114	SER	2.8
1	A	179	TYR	2.7
1	A	205	GLN	2.7
1	B	170	LYS	2.7
1	A	198	SER	2.7
1	B	148	ASN	2.7
1	B	138	HIS	2.7
1	A	253	ASN	2.7
1	A	100	GLU	2.6
1	B	95	PRO	2.6
1	B	122	GLU	2.6
1	B	39	GLN	2.6
1	B	173	GLU	2.6
1	B	203	PRO	2.5
1	B	141	ASN	2.5
1	B	133	PHE	2.5
1	A	116	SER	2.5
1	B	178	PHE	2.5
1	B	201	ASP	2.4
1	A	190	GLU	2.4
1	A	247	ASP	2.4
1	A	40	GLN	2.4
1	B	219	GLN	2.3
1	B	46	ILE	2.3
1	B	143	ASN	2.3
1	A	213	ALA	2.3
1	B	137	LEU	2.3
1	B	73	ASN	2.3
1	A	225	GLU	2.2
1	B	167	GLU	2.2
1	B	131	ALA	2.2
1	B	96	ASN	2.2
1	B	135	GLU	2.2
1	B	206	SER	2.2
1	B	62	GLN	2.2
1	A	244	LEU	2.2
1	B	186	ASN	2.2
1	A	145	GLU	2.1
1	A	241	ILE	2.1
1	B	71	SER	2.1
1	B	140	PRO	2.1
1	B	128	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	ASN	2.1
1	B	82	ASN	2.1
1	A	111	ASP	2.1
1	A	39	GLN	2.1
1	A	200	LYS	2.0
1	A	109	LEU	2.0
1	A	202	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.