



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:36 PM UTC

PDB ID : 6K2D / pdb_00006k2d
Title : The crystal structure of GBP1 with LRR domain of IpaH9.8
Authors : Ji, C.G.; Xiao, J.Y.
Deposited on : 2019-05-14
Resolution : 3.60 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

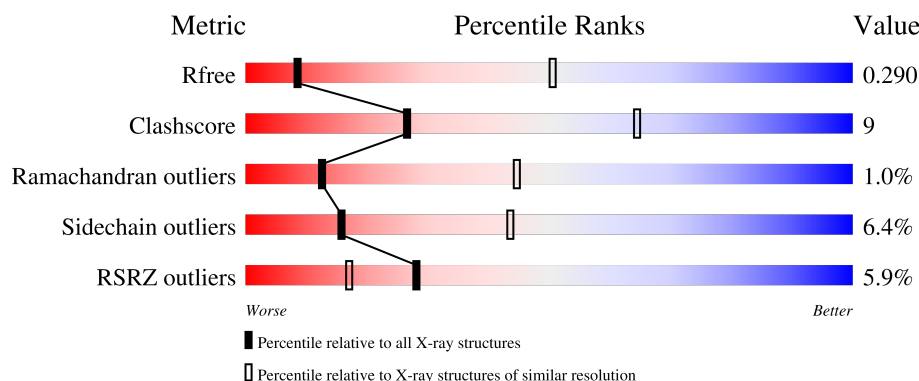
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	481	
2	B	236	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5138 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 Guanylate-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3419	2183	575	643	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P32455
A	0	GLU	-	expression tag	UNP P32455

- Molecule 2 is a protein called E3 ubiquitin-protein ligase ipaH9.8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1719	1091	292	333	3			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	SER	-	expression tag	UNP Q8VSC3
B	18	GLY	-	expression tag	UNP Q8VSC3
B	19	ARG	-	expression tag	UNP Q8VSC3
B	20	PRO	-	expression tag	UNP Q8VSC3
B	21	MET	-	expression tag	UNP Q8VSC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.74Å 211.74Å 56.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.39 – 3.60 48.39 – 3.60	Depositor EDS
% Data completeness (in resolution range)	61.9 (48.39-3.60) 40.5 (48.39-3.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.70 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.240 , 0.287 0.244 , 0.290	Depositor DCC
R_{free} test set	730 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.998	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	5138	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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	0.14	0/3485	0.33	0/4698
2	B	0.13	0/1758	0.35	0/2399
All	All	0.14	0/5243	0.34	0/7097

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	3419	0	3432	59	0
2	B	1719	0	1705	38	0
All	All	5138	0	5137	95	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 (95) 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:205:SER:O	1:A:223:ARG:NH1	2.18	0.76
1:A:20:ARG:NH1	1:A:22:MET:SD	2.64	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TYR:O	1:A:276:ASN:ND2	2.24	0.70
1:A:201:TYR:O	1:A:205:SER:HB2	1.93	0.68
2:B:194:SER:HB2	2:B:216:LEU:HA	1.76	0.67
1:A:126:PHE:H	1:A:176:PRO:HB2	1.58	0.67
2:B:107:ASN:OD1	2:B:127:ASN:ND2	2.24	0.66
2:B:162:LEU:HB3	2:B:186:TYR:HB3	1.77	0.65
2:B:145:SER:HB3	2:B:165:THR:HG22	1.79	0.65
1:A:418:LEU:HD22	1:A:439:LYS:HD2	1.80	0.64
1:A:279:THR:HG21	1:A:287:GLN:HB3	1.81	0.61
2:B:132:LEU:HD21	2:B:144:ILE:HG21	1.84	0.59
1:A:133:THR:O	1:A:201:TYR:OH	2.19	0.58
1:A:127:VAL:HG22	1:A:179:VAL:HB	1.86	0.58
2:B:85:SER:O	2:B:87:ASN:ND2	2.36	0.58
2:B:122:LEU:HD23	2:B:142:MET:HE3	1.86	0.57
2:B:194:SER:O	2:B:194:SER:OG	2.15	0.57
1:A:473:ASP:O	1:A:477:GLN:HG2	2.03	0.57
1:A:50:GLY:O	1:A:183:ARG:NH2	2.33	0.56
1:A:419:GLU:O	1:A:423:LYS:HB2	2.06	0.56
2:B:27:PHE:HD1	2:B:51:LYS:HE2	1.71	0.56
1:A:201:TYR:O	1:A:205:SER:CB	2.54	0.55
2:B:106:SER:HA	2:B:126:HIS:HB2	1.88	0.55
2:B:163:ARG:HE	2:B:187:PHE:HE2	1.56	0.54
1:A:10:PRO:HB3	1:A:81:TRP:HB2	1.89	0.54
1:A:40:VAL:HB	1:A:123:SER:HA	1.90	0.54
2:B:216:LEU:HB2	2:B:221:LEU:HD22	1.90	0.53
1:A:147:GLU:OE2	2:B:146:TYR:OH	2.24	0.53
1:A:110:GLN:OE1	1:A:110:GLN:N	2.42	0.53
1:A:39:VAL:HG22	1:A:279:THR:HA	1.91	0.53
2:B:52:GLU:O	2:B:56:ASN:ND2	2.32	0.53
1:A:357:HIS:NE2	1:A:392:ARG:HB2	2.24	0.52
2:B:34:GLU:HA	2:B:43:ARG:HG3	1.90	0.52
2:B:227:LEU:O	2:B:230:SER:OG	2.23	0.51
1:A:361:GLU:HG3	1:A:388:LEU:HD23	1.93	0.50
1:A:351:GLN:O	1:A:355:ASP:HB2	2.11	0.50
1:A:334:HIS:O	1:A:334:HIS:ND1	2.45	0.49
1:A:182:LEU:HD12	1:A:185:PHE:CE2	2.48	0.48
2:B:109:LEU:H	2:B:127:ASN:HD22	1.61	0.48
1:A:202:LEU:HD13	1:A:235:CYS:HB2	1.96	0.48
1:A:357:HIS:CD2	1:A:392:ARG:HB2	2.48	0.48
2:B:46:ALA:HB2	2:B:66:LEU:HD13	1.96	0.48
1:A:37:PRO:HA	1:A:289:ASN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:HB1	1:A:152:ILE:HD11	1.96	0.48
1:A:124:SER:C	1:A:176:PRO:HB3	2.39	0.48
2:B:22:THR:OG1	2:B:23:TYR:N	2.46	0.48
1:A:216:ASP:OD1	1:A:216:ASP:N	2.41	0.47
2:B:230:SER:HB2	2:B:231:PRO:HD2	1.96	0.47
1:A:147:GLU:OE2	2:B:166:ARG:NH1	2.47	0.47
2:B:71:LEU:HD21	2:B:84:VAL:HG11	1.94	0.47
1:A:51:LYS:NZ	1:A:98:THR:OG1	2.47	0.47
2:B:137:ASP:HA	2:B:156:PRO:HB3	1.97	0.47
1:A:134:ILE:HG13	1:A:182:LEU:HD11	1.97	0.46
1:A:234:LYS:HD3	1:A:272:TYR:CZ	2.50	0.46
1:A:262:PHE:HA	1:A:265:GLN:HB3	1.96	0.46
2:B:99:LEU:HB3	2:B:116:PRO:HG2	1.98	0.46
1:A:299:THR:HG21	1:A:315:ALA:HA	1.97	0.46
1:A:292:ARG:HG2	1:A:319:LEU:HD21	1.98	0.45
2:B:66:LEU:HB2	2:B:68:LEU:HG	1.99	0.45
1:A:439:LYS:HG3	1:A:440:LEU:N	2.32	0.45
1:A:85:HIS:HA	1:A:93:LEU:HD22	1.98	0.45
1:A:41:VAL:HB	1:A:125:THR:HG23	1.98	0.44
1:A:378:HIS:O	1:A:382:LYS:NZ	2.48	0.44
1:A:121:LEU:HD21	1:A:152:ILE:HG21	2.00	0.44
1:A:292:ARG:HG2	1:A:319:LEU:HD11	2.00	0.44
2:B:187:PHE:HB3	2:B:210:HIS:HB2	1.99	0.44
1:A:433:TYR:HD2	1:A:475:ILE:HG22	1.82	0.43
1:A:439:LYS:O	1:A:443:LEU:HB2	2.19	0.43
1:A:108:ASP:HB2	1:A:110:GLN:OE1	2.18	0.43
2:B:24:ALA:HA	2:B:27:PHE:HD2	1.84	0.43
2:B:28:SER:O	2:B:32:LYS:HG3	2.19	0.43
2:B:22:THR:OG1	2:B:25:ASP:OD1	2.29	0.43
2:B:187:PHE:HB3	2:B:210:HIS:CG	2.53	0.43
2:B:34:GLU:O	2:B:43:ARG:NE	2.52	0.42
1:A:128:TYR:O	1:A:181:THR:OG1	2.34	0.42
2:B:132:LEU:HD13	2:B:149:ILE:HG12	2.02	0.42
1:A:422:VAL:HG11	1:A:471:MET:HE3	2.01	0.42
1:A:230:PHE:CD1	1:A:230:PHE:N	2.87	0.42
2:B:217:SER:HB3	2:B:220:ALA:HB3	2.02	0.41
2:B:155:LEU:HD12	2:B:175:PHE:CD2	2.55	0.41
1:A:88:LYS:HG3	1:A:89:PRO:HD2	2.02	0.41
1:A:290:GLY:O	1:A:293:LEU:N	2.54	0.41
2:B:210:HIS:CD2	2:B:210:HIS:N	2.89	0.41
1:A:39:VAL:HG11	1:A:277:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PHE:N	1:A:230:PHE:HD1	2.18	0.41
1:A:289:ASN:OD1	1:A:292:ARG:HD2	2.21	0.41
1:A:16:ASN:ND2	1:A:108:ASP:OD1	2.52	0.41
1:A:128:TYR:HE1	1:A:130:SER:HB3	1.85	0.41
1:A:238:PHE:HE1	1:A:266:VAL:HA	1.85	0.41
2:B:43:ARG:HG2	2:B:44:ASP:N	2.36	0.41
1:A:313:GLU:O	1:A:317:LEU:HG	2.21	0.40
1:A:38:MET:HA	1:A:92:ILE:O	2.21	0.40
1:A:51:LYS:HE2	1:A:51:LYS:HB3	1.88	0.40
2:B:172:LEU:HD23	2:B:172:LEU:HA	1.81	0.40
2:B:129:LEU:HB2	2:B:149:ILE:HD11	2.03	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	418/481 (87%)	365 (87%)	50 (12%)	3 (1%)	18	51
2	B	210/236 (89%)	176 (84%)	31 (15%)	3 (1%)	9	38
All	All	628/717 (88%)	541 (86%)	81 (13%)	6 (1%)	12	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	PRO
1	A	457	ALA
2	B	42	GLU
2	B	133	PRO
1	A	286	ILE
2	B	197	PRO

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	381/428 (89%)	360 (94%)	21 (6%)	19	47
2	B	199/218 (91%)	183 (92%)	16 (8%)	11	37
All	All	580/646 (90%)	543 (94%)	37 (6%)	16	43

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	75	THR
1	A	104	VAL
1	A	109	ASN
1	A	125	THR
1	A	142	LEU
1	A	185	PHE
1	A	202	LEU
1	A	208	LEU
1	A	216	ASP
1	A	234	LYS
1	A	259	ASP
1	A	276	ASN
1	A	282	LEU
1	A	288	VAL
1	A	339	MET
1	A	411	LEU
1	A	434	ARG
1	A	435	LEU
1	A	455	ILE
1	A	478	THR
2	B	44	ASP
2	B	108	LYS
2	B	123	GLN
2	B	124	VAL
2	B	150	VAL
2	B	159	LEU

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Mol	Chain	Res	Type
2	B	165	THR
2	B	166	ARG
2	B	186	TYR
2	B	187	PHE
2	B	189	ASP
2	B	194	SER
2	B	206	GLU
2	B	210	HIS
2	B	213	ASP
2	B	221	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	111	ASN
1	A	264	GLN
2	B	67	ASN
2	B	83	ASN
2	B	205	ASN
2	B	210	HIS

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	428/481 (88%)	0.49	26 (6%) 27 16	9, 66, 112, 131	0
2	B	214/236 (90%)	0.65	12 (5%) 30 18	7, 40, 118, 141	0
All	All	642/717 (89%)	0.55	38 (5%) 28 17	7, 57, 115, 141	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	GLU	5.5
1	A	381	GLN	4.5
2	B	196	ILE	4.3
1	A	198	PRO	3.7
1	A	377	ASP	3.6
2	B	195	HIS	3.6
1	A	285	GLY	3.5
1	A	53	TYR	3.5
2	B	64	ASP	3.4
1	A	386	ALA	3.2
1	A	217	GLU	3.1
2	B	22	THR	3.1
2	B	32	LYS	3.0
2	B	227	LEU	3.0
1	A	448	TYR	2.9
2	B	200	ILE	2.7
1	A	459	GLU	2.7
1	A	432	GLY	2.6
1	A	464	TYR	2.6
1	A	400	GLN	2.4
1	A	127	VAL	2.4
1	A	51	LYS	2.4
1	A	397	LYS	2.4
1	A	26	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	270	CYS	2.4
1	A	108	ASP	2.4
2	B	164	ALA	2.3
1	A	393	ASP	2.3
2	B	199	SER	2.2
1	A	15	GLU	2.2
1	A	184	ASP	2.2
1	A	347	THR	2.2
2	B	43	ARG	2.1
1	A	269	PHE	2.1
1	A	209	LYS	2.1
2	B	142	MET	2.1
2	B	28	SER	2.0
1	A	141	GLN	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 oligosaccharides 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.