



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:02 PM UTC

PDB ID : 6QHD / pdb_00006qhd
Title : Lysine acetylated and tyrosine phosphorylated STAT3 in a complex with DNA
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Deposited on : 2019-01-16
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

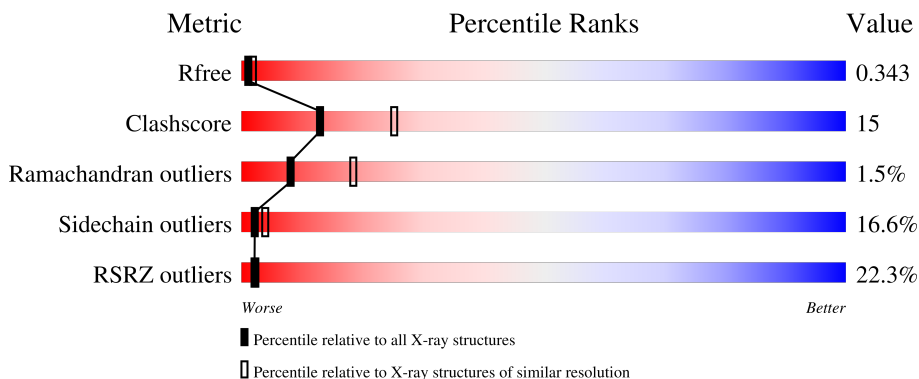
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	596	21% 54% 27% 6% 11%
1	B	596	20% 55% 25% 8% 11%
2	C	18	72% 17% 11%
3	D	18	56% 44%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9454 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 Signal transducer and activator of transcription 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	P	S	0	1	0
			4310	2756	728	796	1	29			
1	B	532	Total	C	N	O	P	S	0	0	0
			4323	2767	731	797	1	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	631	SER	LYS	conflict	UNP P40763
B	631	SER	LYS	conflict	UNP P40763

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*GP*AP*TP*TP*TP*AP*CP*GP*GP*GP*AP*AP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	P		0	0	0
			372	178	74	103	17				

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*GP*CP*AP*TP*TP*TP*CP*CP*CP*GP*TP*AP*AP*AP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	18	Total	C	N	O	P		0	0	0
			360	175	59	109	17				

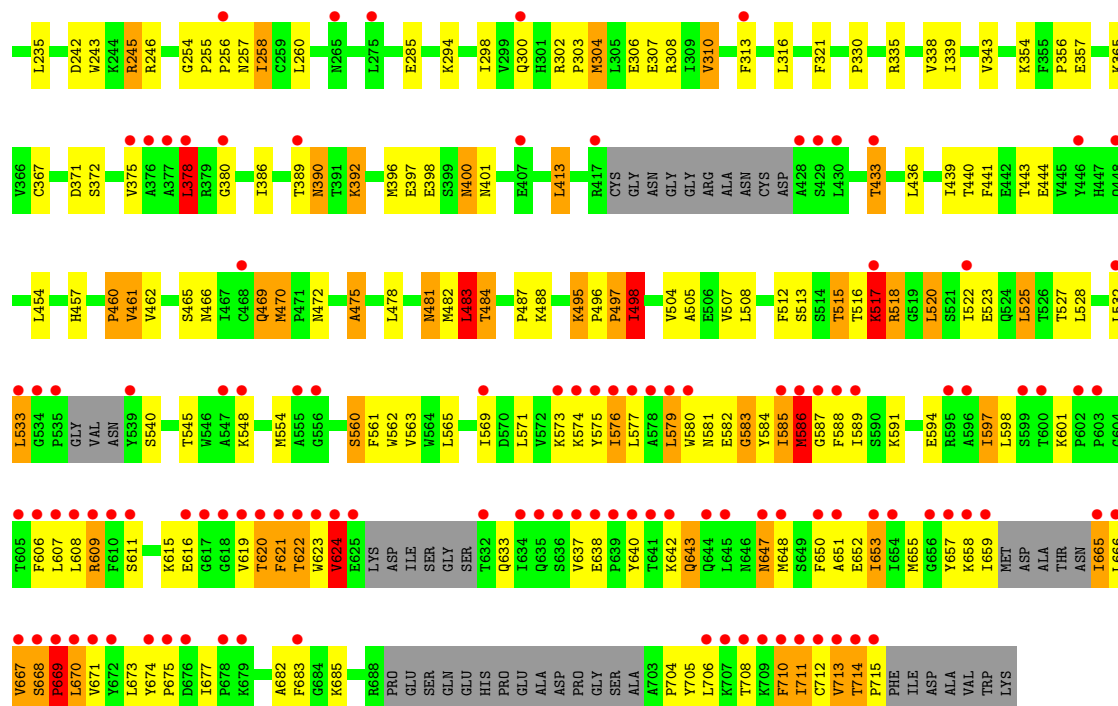
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	36	Total	O	0	0
			36	36		

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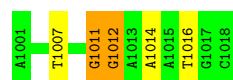
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	6	Total 6	O 6	0	0
4	D	5	Total 5	O 5	0	0



• Molecule 2: DNA (5'-D(*AP*AP*GP*AP*TP*TP*TP*AP*CP*GP*GP*GP*AP*AP*AP*TP*GP*C)-3')

Chain C: 72% 17% 11%



• Molecule 3: DNA (5'-D(*TP*GP*CP*AP*TP*TP*TP*CP*CP*CP*GP*TP*AP*AP*AP*TP*CP*T)-3')

Chain D: 56% 44%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	175.49Å 175.49Å 79.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.85) 100.0 (50.00-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.294 , 0.343 0.294 , 0.343	Depositor DCC
R_{free} test set	2781 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9454	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 98.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6998e-11. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

5.1 Standard geometry

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

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	1.32	11/4364 (0.3%)	1.40	34/5886 (0.6%)
1	B	1.33	13/4374 (0.3%)	1.38	33/5900 (0.6%)
2	C	0.72	0/419	1.29	4/646 (0.6%)
3	D	0.66	0/401	1.36	6/616 (1.0%)
All	All	1.28	24/9558 (0.3%)	1.38	77/13048 (0.6%)

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	439	ILE	C-O	-7.31	1.15	1.24
1	A	439	ILE	C-O	-7.28	1.15	1.24
1	A	365	LYS	C-O	-6.51	1.16	1.24
1	B	668	SER	N-CA	6.29	1.55	1.46
1	B	668	SER	CA-C	6.23	1.60	1.52

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	671	VAL	CB-CA-C	-9.08	102.97	111.05
1	B	624	VAL	N-CA-C	9.01	121.78	108.45
1	B	667	VAL	N-CA-C	8.81	121.70	109.45
1	A	671	VAL	CB-CA-C	-8.62	103.38	111.05
1	B	586	MET	N-CA-C	-8.20	101.40	111.40

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	4310	0	4367	140	0
1	B	4323	0	4391	141	0
2	C	372	0	204	2	0
3	D	360	0	207	2	0
4	A	42	0	0	2	0
4	B	36	0	0	1	0
4	C	6	0	0	0	0
4	D	5	0	0	0	0
All	All	9454	0	9169	277	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 15.

The worst 5 of 277 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:517:LYS:HE2	1:A:577:LEU:CD2	1.70	1.20
1:A:656:GLY:O	1:A:711:ILE:CD1	1.96	1.13
1:A:711:ILE:HG12	1:A:713:VAL:HG13	1.33	1.10
1:A:517:LYS:HE2	1:A:577:LEU:HD23	1.19	1.09
1:B:505:ALA:HB1	1:B:525:LEU:HD11	1.46	0.96

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	515/596 (86%)	488 (95%)	20 (4%)	7 (1%)	9	19
1	B	516/596 (87%)	485 (94%)	23 (4%)	8 (2%)	7	17
All	All	1031/1192 (86%)	973 (94%)	43 (4%)	15 (2%)	8	18

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	GLY
1	A	669	PRO
1	A	704	PRO
1	B	497	PRO
1	B	669	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	483/532 (91%)	401 (83%)	82 (17%)	2	3
1	B	484/532 (91%)	406 (84%)	78 (16%)	2	4
All	All	967/1064 (91%)	807 (84%)	160 (16%)	2	4

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	444	GLU
1	B	621	PHE
1	B	484	THR
1	B	525	LEU
1	B	643	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	141	GLN

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Mol	Chain	Res	Type
1	B	543	GLN
1	B	288	GLN
1	B	647	ASN
1	B	469	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	ALY	B	685	1	10,11,12	0.79	0	7,12,14	2.46	4 (57%)
1	ALY	A	685	1	10,11,12	0.85	0	7,12,14	2.29	3 (42%)
1	PTR	B	705	1	15,16,17	2.78	7 (46%)	17,22,24	2.27	6 (35%)
1	PTR	A	705	1	15,16,17	2.81	8 (53%)	17,22,24	1.91	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	B	685	1	-	2/9/10/12	-
1	ALY	A	685	1	-	3/9/10/12	-
1	PTR	B	705	1	-	3/10/11/13	0/1/1/1
1	PTR	A	705	1	-	1/10/11/13	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	705	PTR	CE1-CD1	5.26	1.47	1.38
1	B	705	PTR	CE2-CD2	5.22	1.47	1.38
1	A	705	PTR	CE2-CD2	4.99	1.46	1.38
1	B	705	PTR	CE1-CD1	4.88	1.46	1.38
1	B	705	PTR	CE1-CZ	4.09	1.46	1.38

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	705	PTR	CE2-CZ-CE1	-4.94	112.95	120.16
1	B	705	PTR	CD1-CE1-CZ	4.51	124.88	119.73
1	A	705	PTR	CE2-CZ-CE1	-4.02	114.30	120.16
1	A	705	PTR	CD1-CE1-CZ	3.83	124.11	119.73
1	B	685	ALY	CD-CE-NZ	3.68	122.51	112.20

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	705	PTR	O-C-CA-CB
1	B	705	PTR	O-C-CA-CB
1	A	685	ALY	OH-CH-NZ-CE
1	A	685	ALY	CH3-CH-NZ-CE
1	B	685	ALY	OH-CH-NZ-CE

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	528/596 (88%)	1.14	125 (23%) 2 2	63, 100, 170, 194	1 (0%)
1	B	530/596 (88%)	1.10	119 (22%) 2 2	71, 100, 173, 225	0
2	C	18/18 (100%)	-0.15	0 100 100	76, 92, 115, 119	0
3	D	18/18 (100%)	-0.34	0 100 100	72, 89, 112, 116	0
All	All	1094/1228 (89%)	1.08	244 (22%) 2 2	63, 99, 171, 225	1 (0%)

The worst 5 of 244 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	623	TRP	9.3
1	B	195	VAL	7.3
1	A	666	LEU	7.3
1	B	666	LEU	7.3
1	B	579	LEU	7.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	ALY	B	685	12/13	0.49	0.21	142,145,146,148	0
1	ALY	A	685	12/13	0.56	0.19	140,144,146,147	0
1	PTR	B	705	16/17	0.87	0.14	153,160,168,173	0
1	PTR	A	705	16/17	0.88	0.15	147,157,166,170	0

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.