



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:05 PM UTC

PDB ID : 5OEN / pdb_00005oen
Title : Crystal Structure of STAT2 in complex with IRF9
Authors : Rengachari, S.; Panne, D.
Deposited on : 2017-07-09
Resolution : 2.92 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

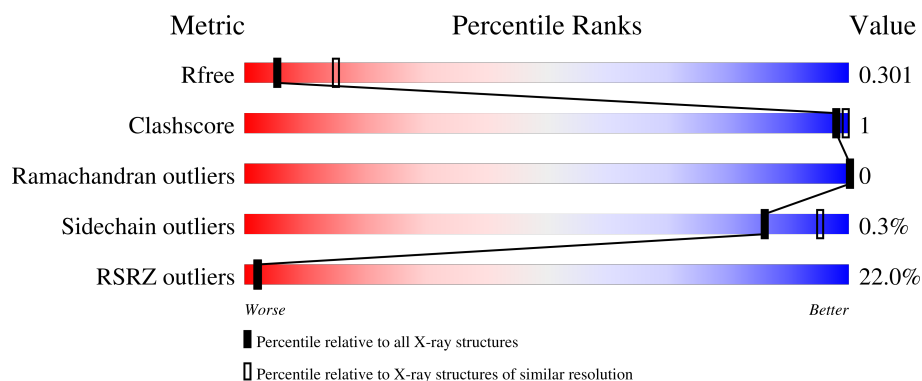
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	171	22% 94%
2	B	175	21% 97%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5436 atoms, of which 2719 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 Interferon regulatory factor 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	165	Total	C	H	N	O	S	0	0	0
			2595	837	1289	225	238	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	347	ALA	GLU	engineered mutation	UNP Q61179
A	348	ALA	GLU	engineered mutation	UNP Q61179

- Molecule 2 is a protein called Signal transducer and activator of transcription.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	171	Total	C	H	N	O	S	0	0	0
			2822	884	1430	249	253	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	242	ALA	GLN	engineered mutation	UNP Q3UDU1
B	243	ALA	LYS	engineered mutation	UNP Q3UDU1

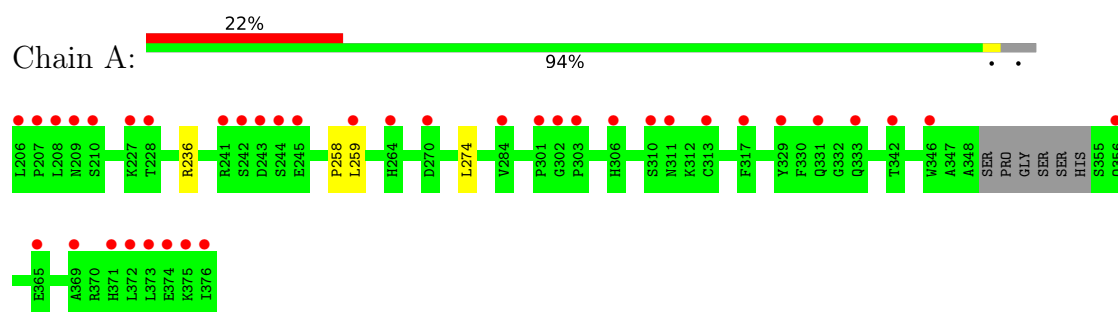
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	7	Total	O	0	0
			7	7		

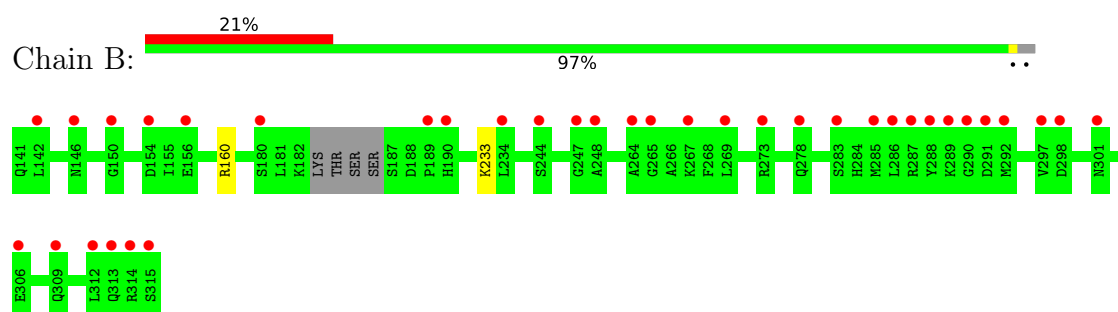
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Interferon regulatory factor 9



- Molecule 2: Signal transducer and activator of transcription



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	30.60Å 124.04Å 51.03Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	32.12 – 2.92 32.12 – 2.92	Depositor EDS
% Data completeness (in resolution range)	88.3 (32.12-2.92) 88.9 (32.12-2.92)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.255 , 0.307 0.248 , 0.301	Depositor DCC
R_{free} test set	767 reflections (7.37%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	5436	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.64% 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

5.1 Standard geometry

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	0.11	0/1342	0.27	0/1827
2	B	0.10	0/1412	0.25	0/1898
All	All	0.10	0/2754	0.26	0/3725

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

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	1306	1289	1291	3	0
2	B	1392	1430	1432	1	0
3	A	12	0	0	0	0
3	B	7	0	0	1	0
All	All	2717	2719	2723	4	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 1.

All (4) 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:B:160:ARG:NH1	3:B:401:HOH:O	1.94	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:PRO:O	1:A:259:LEU:HB3	2.21	0.41
1:A:236:ARG:HD3	1:A:274:LEU:HD21	2.03	0.41
1:A:258:PRO:O	1:A:259:LEU:CB	2.69	0.41

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	161/171 (94%)	152 (94%)	9 (6%)	0	100	100
2	B	167/175 (95%)	163 (98%)	4 (2%)	0	100	100
All	All	328/346 (95%)	315 (96%)	13 (4%)	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	146/151 (97%)	146 (100%)	0	100	100
2	B	154/158 (98%)	153 (99%)	1 (1%)	78	92
All	All	300/309 (97%)	299 (100%)	1 (0%)	86	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	233	LYS

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	250	GLN
1	A	263	GLN
2	B	260	GLN
2	B	301	ASN

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

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	165/171 (96%)	1.37	38 (23%) 2 2	15, 33, 79, 121	0
2	B	171/175 (97%)	1.31	36 (21%) 2 2	21, 42, 71, 89	0
All	All	336/346 (97%)	1.34	74 (22%) 2 2	15, 38, 75, 121	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	ILE	7.1
1	A	209	ASN	6.0
2	B	290	GLY	5.9
1	A	311	ASN	5.6
1	A	207	PRO	5.6
1	A	245	GLU	5.4
2	B	288	TYR	4.7
1	A	208	LEU	4.6
2	B	289	LYS	4.4
1	A	310	SER	4.0
2	B	291	ASP	3.9
2	B	247	GLY	3.7
1	A	313	CYS	3.6
1	A	303	PRO	3.4
1	A	373	LEU	3.3
2	B	297	VAL	3.3
2	B	287	ARG	3.3
1	A	375	LYS	3.2
1	A	374	GLU	3.2
2	B	315	SER	3.2
1	A	329	TYR	3.2
1	A	206	LEU	3.2
2	B	313	GLN	3.1
1	A	317	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	301	ASN	3.0
1	A	302	GLY	3.0
2	B	146	ASN	3.0
1	A	210	SER	3.0
1	A	333	GLN	2.9
1	A	301	PRO	2.9
1	A	241	ARG	2.9
1	A	371	HIS	2.9
1	A	284	VAL	2.8
2	B	248	ALA	2.8
2	B	244	SER	2.8
1	A	264	HIS	2.7
2	B	292	MET	2.7
2	B	283	SER	2.7
2	B	286	LEU	2.7
1	A	243	ASP	2.6
2	B	189	PRO	2.6
2	B	269	LEU	2.6
1	A	259	LEU	2.4
2	B	190	HIS	2.4
2	B	267	LYS	2.4
2	B	264	ALA	2.4
1	A	365	GLU	2.4
2	B	278	GLN	2.4
1	A	270	ASP	2.3
2	B	234	LEU	2.3
1	A	242	SER	2.3
1	A	228	THR	2.3
2	B	265	GLY	2.3
2	B	154	ASP	2.3
1	A	342	THR	2.3
1	A	227	LYS	2.2
1	A	331	GLN	2.2
2	B	314	ARG	2.2
2	B	142	LEU	2.2
2	B	306	GLU	2.2
2	B	273	ARG	2.2
1	A	356	GLN	2.1
2	B	298	ASP	2.1
1	A	346	TRP	2.1
2	B	150	GLY	2.1
2	B	180	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	309	GLN	2.1
1	A	306	HIS	2.1
2	B	285	MET	2.1
1	A	244	SER	2.1
2	B	312	LEU	2.1
1	A	372	LEU	2.0
1	A	369	ALA	2.0
2	B	156	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.