



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:04 AM GMT

PDB ID : 3D7U
Title : Structural basis for the recognition of c-Src by its inactivator Csk
Authors : Levinson, N.M.; Seeliger, M.A.; Cole, P.A.; Kuriyan, J.
Deposited on : 2008-05-21
Resolution : 4.11 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

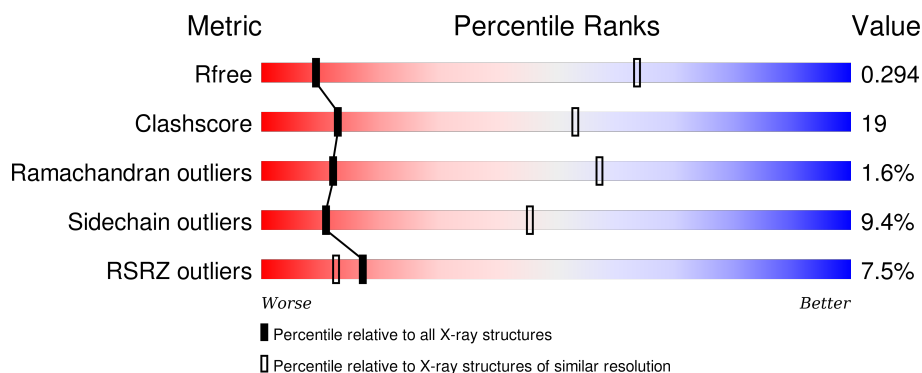
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.11 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}	91344	1020 (4.62-3.60)
Clashscore	102246	1119 (4.62-3.60)
Ramachandran outliers	100387	1065 (4.62-3.60)
Sidechain outliers	100360	1051 (4.62-3.60)
RSRZ outliers	91569	1024 (4.62-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	263	<div> <div>14%</div> <div>70% 24% . .</div> </div>
1	C	263	<div> <div>10%</div> <div>71% 23% . .</div> </div>
2	B	277	<div> <div>2%</div> <div>56% 32% . . 7%</div> </div>
2	D	277	<div> <div>4%</div> <div>55% 30% 5% 10%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8153 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 Tyrosine-protein kinase CSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2038	1306	349	370	13			
1	C	257	Total	C	N	O	S	0	0	0
			2038	1306	349	370	13			

- Molecule 2 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2080	1334	347	382	17			
2	D	248	Total	C	N	O	S	0	0	0
			1997	1283	334	363	17			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	257	LYS	-	EXPRESSION TAG	UNP P00523
B	258	ASP	-	EXPRESSION TAG	UNP P00523
B	259	ALA	-	EXPRESSION TAG	UNP P00523
B	524	GLU	-	EXPRESSION TAG	UNP P00523
B	525	PRO	-	EXPRESSION TAG	UNP P00523
B	526	GLN	-	EXPRESSION TAG	UNP P00523
B	527	TYR	-	EXPRESSION TAG	UNP P00523
B	528	GLN	-	EXPRESSION TAG	UNP P00523
B	529	PRO	-	EXPRESSION TAG	UNP P00523
B	530	GLY	-	EXPRESSION TAG	UNP P00523
B	531	GLU	-	EXPRESSION TAG	UNP P00523
B	532	ASN	-	EXPRESSION TAG	UNP P00523
B	533	LEU	-	EXPRESSION TAG	UNP P00523
D	257	LYS	-	EXPRESSION TAG	UNP P00523
D	258	ASP	-	EXPRESSION TAG	UNP P00523
D	259	ALA	-	EXPRESSION TAG	UNP P00523

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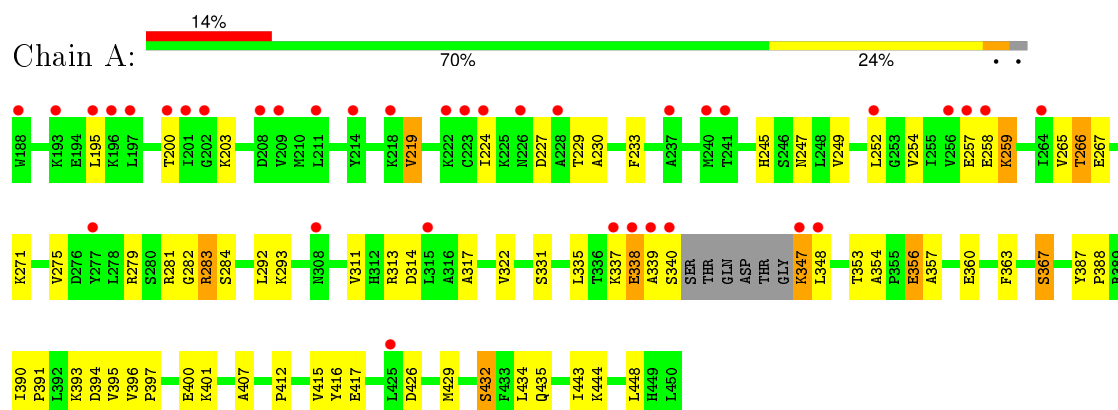
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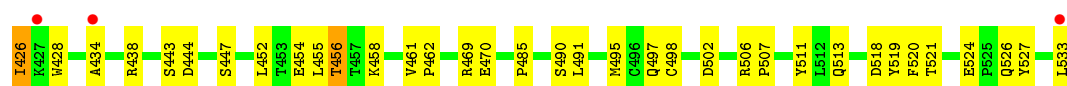
Chain	Residue	Modelled	Actual	Comment	Reference
D	524	GLU	-	EXPRESSION TAG	UNP P00523
D	525	PRO	-	EXPRESSION TAG	UNP P00523
D	526	GLN	-	EXPRESSION TAG	UNP P00523
D	527	TYR	-	EXPRESSION TAG	UNP P00523
D	528	GLN	-	EXPRESSION TAG	UNP P00523
D	529	PRO	-	EXPRESSION TAG	UNP P00523
D	530	GLY	-	EXPRESSION TAG	UNP P00523
D	531	GLU	-	EXPRESSION TAG	UNP P00523
D	532	ASN	-	EXPRESSION TAG	UNP P00523
D	533	LEU	-	EXPRESSION TAG	UNP P00523

3 Residue-property plots [i](#)

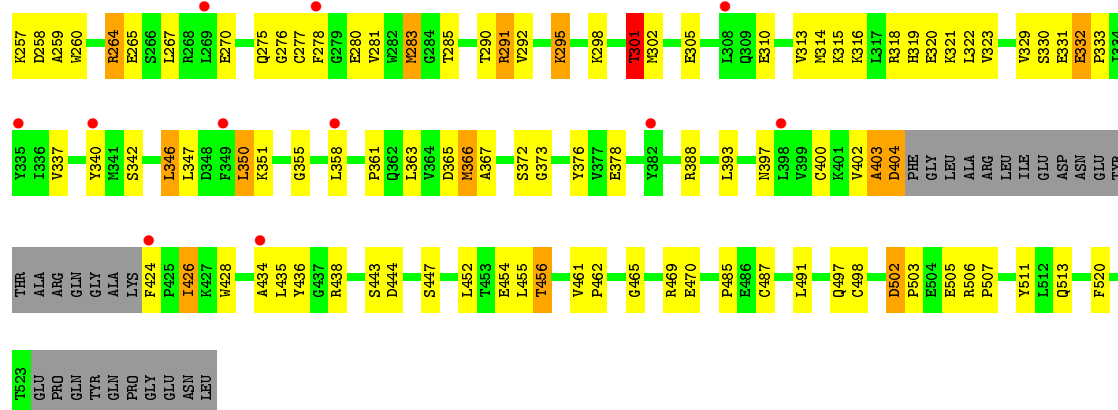
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Tyrosine-protein kinase CSK





● Molecule 2: Proto-oncogene tyrosine-protein kinase Src



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	135.84Å 135.84Å 129.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.87 – 4.11 46.87 – 4.11	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.87-4.11) 98.6 (46.87-4.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.294 , 0.302 0.288 , 0.294	Depositor DCC
R_{free} test set	1053 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	162.2	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 134.6	EDS
Estimated twinning fraction	0.034 for -h,-k,l 0.078 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 20508 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8153	wwPDB-VP
Average B, all atoms (Å ²)	191.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.45	1/2080 (0.0%)	0.64	0/2806
1	C	0.45	1/2080 (0.0%)	0.64	0/2806
2	B	0.76	2/2130 (0.1%)	0.89	8/2882 (0.3%)
2	D	0.82	2/2044 (0.1%)	0.89	6/2765 (0.2%)
All	All	0.64	6/8334 (0.1%)	0.77	14/11259 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	350	LEU	C-N	15.92	1.70	1.34
2	B	350	LEU	C-N	8.27	1.53	1.34
1	A	432	SER	C-O	5.77	1.34	1.23
1	C	432	SER	C-O	5.76	1.34	1.23
2	D	342	SER	C-O	5.71	1.34	1.23

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	350	LEU	CA-C-N	-8.24	99.08	117.20
2	B	350	LEU	CA-C-N	-8.08	99.43	117.20
2	D	365	ASP	CB-CG-OD2	6.89	124.50	118.30
2	B	365	ASP	CB-CG-OD2	6.88	124.49	118.30
2	D	258	ASP	CB-CG-OD2	6.84	124.45	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	350	LEU	Mainchain

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	2038	0	2064	92	9
1	C	2038	0	2064	76	12
2	B	2080	0	2065	103	1
2	D	1997	0	1993	108	4
All	All	8153	0	8186	312	13

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 19.

The worst 5 of 312 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:D:350:LEU:C	2:D:351:LYS:N	1.70	1.44
1:C:279:ARG:HD3	2:D:511:TYR:CE2	1.54	1.41
1:A:279:ARG:HD3	2:B:511:TYR:CE2	1.67	1.29
1:A:400:GLU:OE1	2:D:465:GLY:CA	1.79	1.27
1:C:279:ARG:CD	2:D:511:TYR:CE2	2.18	1.26

The worst 5 of 13 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:401:LYS:O	1:C:438:GLU:CD[3_664]	0.35	1.85
1:A:401:LYS:O	1:C:438:GLU:OE2[3_664]	1.08	1.12
1:A:401:LYS:O	1:C:438:GLU:OE1[3_664]	1.30	0.90
1:A:401:LYS:C	1:C:438:GLU:OE1[3_664]	1.52	0.68
1:A:401:LYS:C	1:C:438:GLU:CD[3_664]	1.54	0.66

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	253/263 (96%)	237 (94%)	13 (5%)	3 (1%)	16	62
1	C	253/263 (96%)	237 (94%)	13 (5%)	3 (1%)	16	62
2	B	252/277 (91%)	219 (87%)	28 (11%)	5 (2%)	9	54
2	D	242/277 (87%)	209 (86%)	28 (12%)	5 (2%)	9	52
All	All	1000/1080 (93%)	902 (90%)	82 (8%)	16 (2%)	12	57

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	ALA
1	A	395	VAL
2	B	403	ALA
1	C	339	ALA
1	C	395	VAL

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	220/225 (98%)	210 (96%)	10 (4%)	34	71
1	C	220/225 (98%)	209 (95%)	11 (5%)	30	69
2	B	225/239 (94%)	194 (86%)	31 (14%)	4	29
2	D	216/239 (90%)	185 (86%)	31 (14%)	4	27
All	All	881/928 (95%)	798 (91%)	83 (9%)	11	45

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	470	GLU
1	C	283	ARG
2	D	447	SER
2	B	491	LEU
1	C	219	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	526	GLN
2	B	532	ASN
1	C	442	HIS
2	B	474	GLN
1	C	446	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 carbohydrates 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	257/263 (97%)	0.89	36 (14%) 4 4	143, 178, 256, 262	0
1	C	257/263 (97%)	0.58	25 (9%) 10 8	149, 189, 243, 252	0
2	B	258/277 (93%)	0.39	5 (1%) 70 60	140, 182, 212, 232	0
2	D	248/277 (89%)	0.45	11 (4%) 38 29	143, 198, 221, 229	0
All	All	1020/1080 (94%)	0.58	77 (7%) 17 13	140, 186, 244, 262	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	224	ILE	8.0
1	A	209	VAL	7.1
1	A	222	LYS	6.4
1	A	195	LEU	5.2
1	A	252	LEU	5.0

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 carbohydrates 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.