wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 03:23 AM EDT

PDB ID	:	1K6O
Title	:	Crystal Structure of a Ternary SAP-1/SRF/c-fos SRE DNA Complex
Authors	:	Mo, Y.; Ho, W.; Johnston, K.; Marmorstein, R.
Deposited on	:	2001-10-16
Resolution	:	3.19 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 (i) 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 (i)) were used in the production of this report:

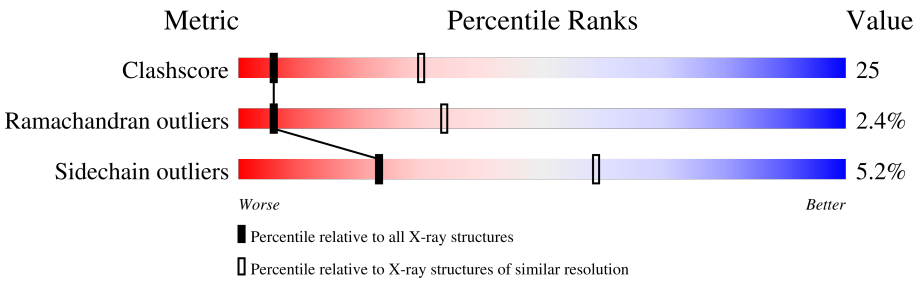
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	23	39% 61%
2	E	23	39% 61%
3	A	93	51% 42% • •
4	B	103	42% 38% • 17%
4	C	103	41% 37% • 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2957 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 DNA chain called 5'-D(*CP*AP*CP*AP*GP*GP*AP*TP*GP*TP*CP*CP*AP*TP*AP*TP*TP*AP*GP*GP*AP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	D	23	470	225	90	133	22	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	23	467	225	81	139	22	0	0	0

- Molecule 3 is a protein called ETS-domain protein ELK-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	89	745	491	129	122	3	0	0	0

- Molecule 4 is a protein called Serum response factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	85	641	407	114	116	4	0	0	0
4	C	84	634	402	109	119	4	0	0	0

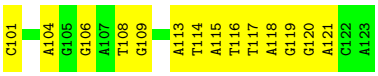
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

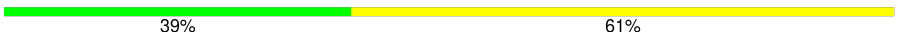
• Molecule 1: 5'-D(*CP*AP*CP*AP*GP*GP*AP*TP*GP*TP*CP*CP*AP*TP*AP*TP*TP*AP*GP*GP*AP*CP*A)-3'

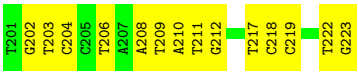
Chain D:



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

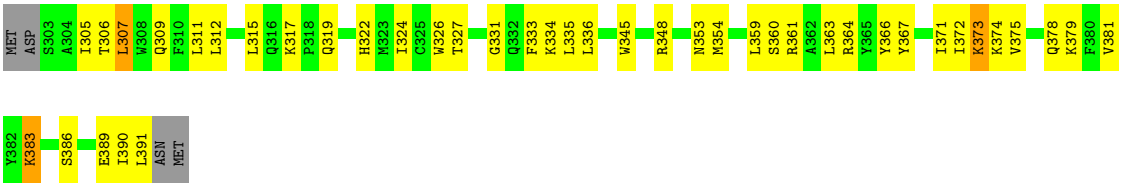
Chain E:





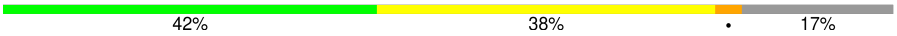
• Molecule 3: ETS-domain protein ELK-4

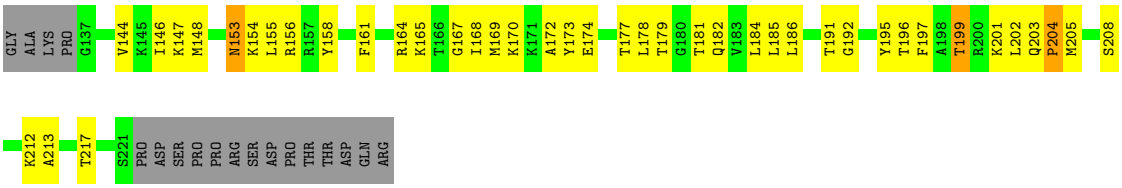
Chain A:



• Molecule 4: Serum response factor

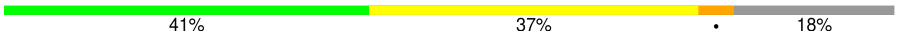
Chain B:

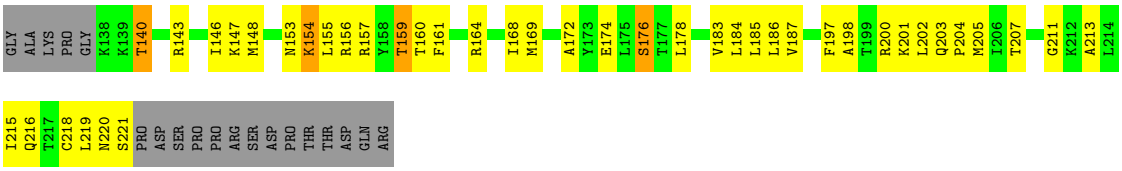




• Molecule 4: Serum response factor

Chain C:


41%
37%
•
18%


GLY ALA LYS PRO GLY K138 K139 T140 R143 I146 K147 M148 N153 K154 L155 R156 R157 Y158 T159 T160 F161 R164 I168 M169 A172 Y173 E174 L175 S176 T177 L178 V183 L184 L185 L186 V187 F197 A198 T199 R200 K201 L202 Q203 P204 M205 I206 T207 G211 K212 A213 L214
I215 Q216 T217 C218 L219 N220 S221 PRO ASP SER PRO PRO ARG SER ASP PRO THR THR ASP GLN ARG

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	161.78Å 161.78Å 41.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.19	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.19)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2957	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

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	D	0.48	0/528	0.70	0/813
2	E	0.53	0/522	0.74	0/804
3	A	0.43	0/764	0.64	0/1032
4	B	0.41	0/647	0.62	0/870
4	C	0.40	0/641	0.64	0/864
All	All	0.45	0/3102	0.67	0/4383

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	D	470	0	260	19	0
2	E	467	0	263	18	0
3	A	745	0	757	43	0
4	B	641	0	661	42	0
4	C	634	0	644	41	0
All	All	2957	0	2585	139	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 25.

The worst 5 of 139 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:E:208:DA:H2"	2:E:209:DT:H5"	1.44	0.99
1:D:118:DA:H5"	4:C:164:ARG:HH11	1.33	0.91
2:E:209:DT:H2"	2:E:210:DA:C8	2.05	0.90
2:E:203:DT:H2"	2:E:204:DC:H5'	1.54	0.90
2:E:202:DG:H2"	2:E:203:DT:O5'	1.76	0.84

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
3	A	87/93 (94%)	70 (80%)	15 (17%)	2 (2%)	6 34
4	B	83/103 (81%)	69 (83%)	12 (14%)	2 (2%)	6 34
4	C	82/103 (80%)	64 (78%)	16 (20%)	2 (2%)	6 34
All	All	252/299 (84%)	203 (81%)	43 (17%)	6 (2%)	6 34

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	154	LYS
3	A	353	ASN
3	A	319	GLN
4	B	192	GLY
4	B	204	PRO

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	
3	A	78/86 (91%)	73 (94%)	5 (6%)	17	52
4	B	66/91 (72%)	63 (96%)	3 (4%)	27	63
4	C	67/91 (74%)	64 (96%)	3 (4%)	27	63
All	All	211/268 (79%)	200 (95%)	11 (5%)	23	59

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	199	THR
4	C	140	THR
4	C	176	SER
4	C	159	THR
3	A	383	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	203	GLN
4	C	193	HIS
4	C	203	GLN
3	A	320	ASN
3	A	316	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 monosaccharides 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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.