Full wwPDB X-ray Structure Validation Report (i)

Mar 22, 2016 – 03:49 AM EDT

PDB ID	:	4XCI
Title	:	Crystal structure of a hexadecameric TF55 complex from S. solfataricus, crystal form II
Authors	:	Stewart, A.G.; Chaston, J.J.; Smits, C.; Stock, D.
Deposited on	:	2014-12-18
Resolution	:	3.00 Å(reported)

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

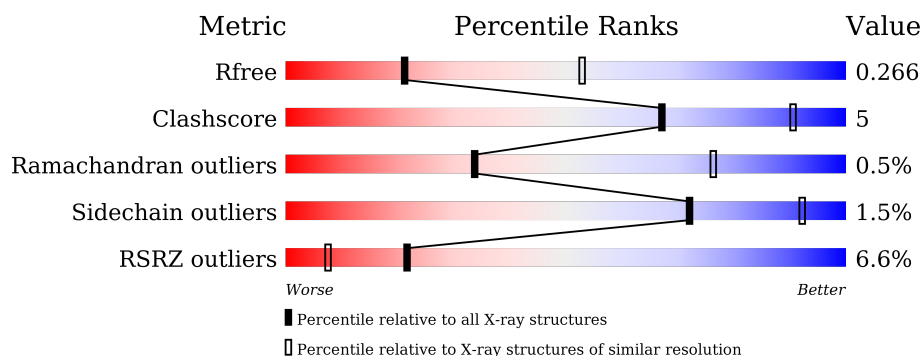|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 3.00 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	Percentile Ranks	Value
Rfree		0.266
Clashscore		5
Ramachandran outliers		0.5%
Sidechain outliers		1.5%
RSRZ outliers		6.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 <=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	B	557	5% — 74% / 6% / 19%
2	A	559	4% — 48% / 6% · / 44%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11773 atoms, of which 6031 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 Thermosome subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	449	Total	C	H	N	O	S	0	0	0
			6986	2154	3577	594	651	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q9V2T8
B	2	ARG	-	expression tag	UNP Q9V2T8
B	3	LYS	-	expression tag	UNP Q9V2T8

- Molecule 2 is a protein called Thermosome subunit alpha.

| Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	313	Total	C	H	N	O	S	0	0	0
			4787	1476	2454	397	454	6			

3 Residue-property plots ⓘ

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: Thermosome subunit beta
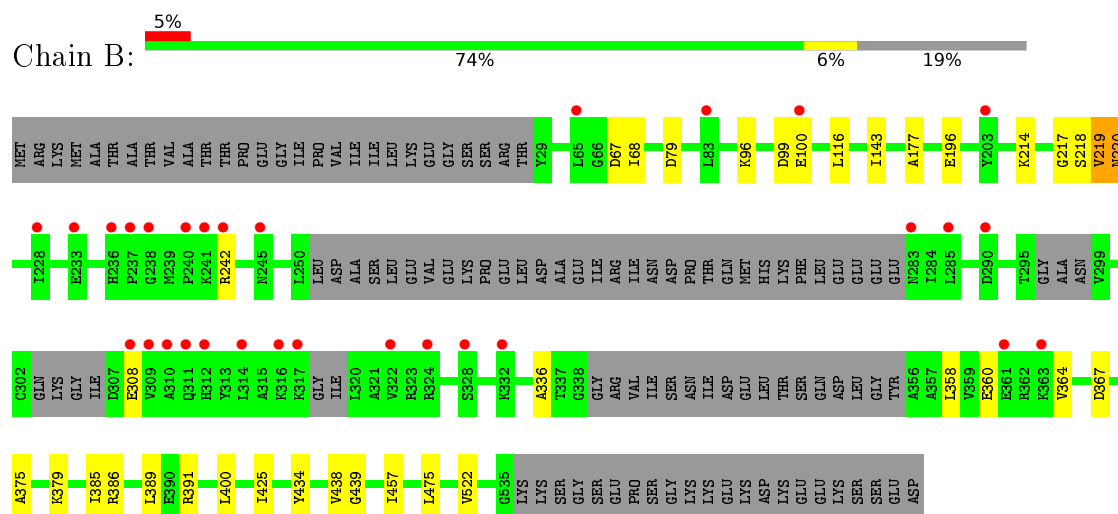
- Molecule 2: Thermosome subunit alpha
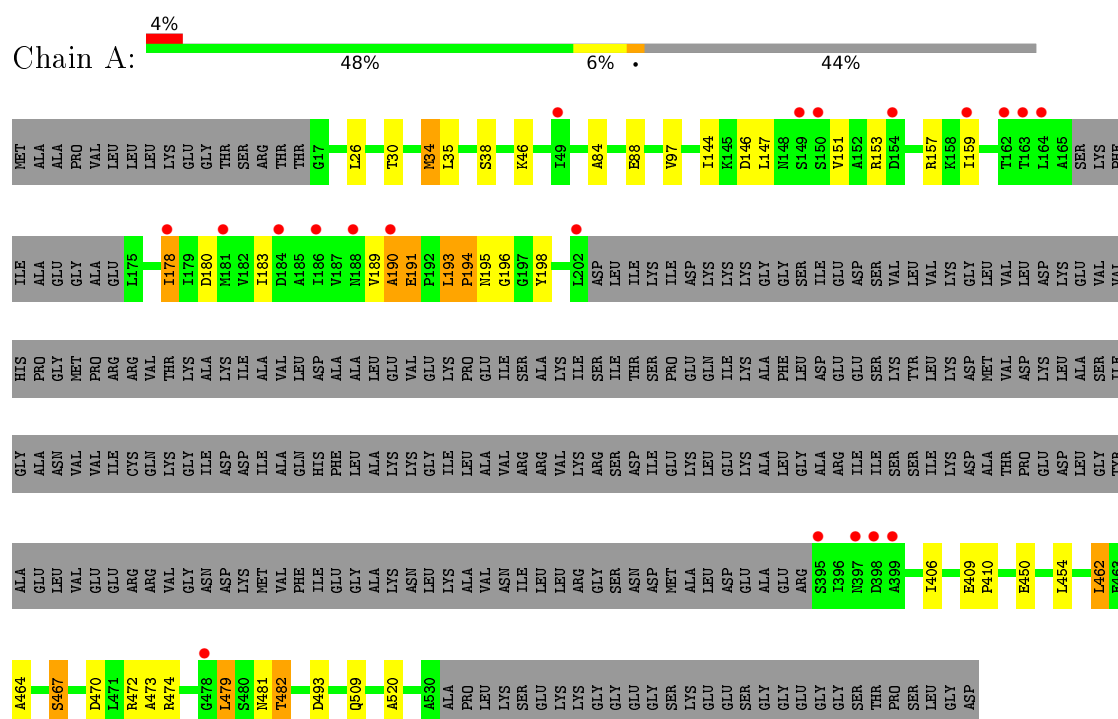
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	148.42Å　　148.42Å　　304.67Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	41.91　−　3.00 41.91　−　3.00	Depositor EDS
% Data completeness (in resolution range)	72.5 (41.91-3.00) 72.5 (41.91-3.00)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.236　,　0.266 0.236　,　0.266	Depositor DCC
R_{free} test set	1273 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 25.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	0 of 24930 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11773	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	B	0.25	0/3439	0.44	0/4636
2	A	0.27	0/2352	0.51	1/3184 (0.0%)
All	All	0.26	0/5791	0.47	1/7820 (0.0%)

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	A	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	191	GLU	N-CA-C	5.38	125.51	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	189	VAL	Peptide
2	A	190	ALA	Peptide
2	A	194	PRO	Peptide

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	B	3409	3577	3571	25	0
2	A	2333	2454	2451	34	0
All	All	5742	6031	6022	56	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 5.

All (56) 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:B:385:ILE:HD11	1:B:400:LEU:HD23	1.75	0.68
1:B:389:LEU:HD21	2:A:84:ALA:HB2	1.75	0.67
1:B:385:ILE:HD11	1:B:400:LEU:CD2	2.26	0.66
2:A:474:ARG:HB2	2:A:482:THR:HG21	1.78	0.65
2:A:193:LEU:HD23	2:A:194:PRO:HD2	1.79	0.65
1:B:242:ARG:NH1	1:B:360:GLU:OE2	2.31	0.64
1:B:214:LYS:NZ	1:B:367:ASP:OD2	2.32	0.63
2:A:462:LEU:HD21	2:A:467:SER:HB2	1.81	0.63
2:A:193:LEU:HD23	2:A:194:PRO:CD	2.31	0.61
2:A:35:LEU:HD12	2:A:97:VAL:HG11	1.82	0.61
2:A:462:LEU:HD21	2:A:467:SER:CB	2.32	0.60
2:A:157:ARG:NH2	2:A:180:ASP:OD1	2.34	0.60
2:A:450:GLU:OE1	2:A:472:ARG:NH2	2.35	0.59
2:A:474:ARG:NH1	2:A:493:ASP:OD1	2.35	0.59
1:B:217:GLY:O	1:B:218:SER:OG	2.15	0.58
1:B:196:GLU:OE1	1:B:379:LYS:NZ	2.38	0.57
1:B:336:ALA:O	1:B:375:ALA:HB1	2.05	0.56
2:A:146:ASP:OD1	2:A:147:LEU:N	2.39	0.56
2:A:474:ARG:CB	2:A:482:THR:HG21	2.35	0.55
1:B:358:LEU:HD21	1:B:360:GLU:OE2	2.06	0.54
2:A:159:ILE:HG21	2:A:406:ILE:HD11	1.90	0.54
2:A:38:SER:OG	2:A:46:LYS:NZ	2.40	0.53
2:A:26:LEU:O	2:A:30:THR:HG23	2.10	0.52
2:A:462:LEU:HD21	2:A:467:SER:OG	2.10	0.52
2:A:479:LEU:O	2:A:481:ASN:N	2.43	0.52
2:A:144:ILE:HD12	2:A:196:GLY:HA3	1.91	0.52
1:B:67:ASP:OD1	1:B:68:ILE:N	2.43	0.52
2:A:144:ILE:HG21	2:A:410:PRO:HG3	1.94	0.50
2:A:462:LEU:C	2:A:462:LEU:HD22	2.32	0.50
1:B:143:ILE:HD11	1:B:434:TYR:CD2	2.46	0.49

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LEU:HD21	2:A:84:ALA:CB	2.41	0.49
2:A:474:ARG:HD2	2:A:482:THR:HG21	1.94	0.49
2:A:144:ILE:CD1	2:A:196:GLY:HA3	2.43	0.48
2:A:144:ILE:O	2:A:198:TYR:OH	2.31	0.48
1:B:219:VAL:HG11	1:B:386:ARG:HB2	1.95	0.48
1:B:425:ILE:CD1	1:B:475:LEU:HB3	2.44	0.48
2:A:470:ASP:O	2:A:473:ALA:HB3	2.14	0.48
1:B:116:LEU:HB2	1:B:522:VAL:HG21	1.96	0.47
2:A:178:ILE:HG22	2:A:178:ILE:O	2.15	0.46
1:B:364:VAL:N	1:B:367:ASP:O	2.48	0.46
1:B:425:ILE:HG13	1:B:457:ILE:CD1	2.47	0.45
1:B:308:GLU:N	1:B:308:GLU:OE1	2.47	0.45
2:A:454:LEU:CD1	2:A:464:ALA:HB1	2.47	0.44
1:B:79:ASP:OD1	1:B:96:LYS:NZ	2.44	0.44
1:B:99:ASP:OD1	1:B:100:GLU:N	2.51	0.43
2:A:147:LEU:O	2:A:153:ARG:NH2	2.49	0.43
1:B:217:GLY:C	1:B:219:VAL:HG23	2.40	0.43
1:B:391:ARG:HH12	2:A:520:ALA:HB1	1.84	0.42
1:B:177:ALA:HB1	1:B:220:ASN:HB2	2.00	0.42
2:A:190:ALA:HB3	2:A:191:GLU:HG3	2.02	0.42
2:A:193:LEU:HD23	2:A:194:PRO:HD3	2.02	0.41
2:A:88:GLU:OE1	2:A:509:GLN:NE2	2.50	0.41
1:B:385:ILE:HD11	1:B:400:LEU:HD22	2.01	0.41
1:B:438:VAL:HG12	1:B:439:GLY:N	2.35	0.41
2:A:34:MET:HE3	2:A:46:LYS:HE2	2.04	0.40
2:A:34:MET:HE2	2:A:35:LEU:HG	2.03	0.40

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	B	437/557 (78%)	413 (94%)	23 (5%)	1 (0%)	52 88
2	A	307/559 (55%)	293 (95%)	11 (4%)	3 (1%)	19 61
All	All	744/1116 (67%)	706 (95%)	34 (5%)	4 (0%)	34 76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	220	ASN
2	A	195	ASN
2	A	178	ILE
2	A	151	VAL

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	B	356/449 (79%)	355 (100%)	1 (0%)	94 98
2	A	248/448 (55%)	240 (97%)	8 (3%)	46 82
All	All	604/897 (67%)	595 (98%)	9 (2%)	72 92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	219	VAL
2	A	34	MET
2	A	183	ILE
2	A	193	LEU
2	A	409	GLU
2	A	462	LEU
2	A	467	SER
2	A	479	LEU
2	A	482	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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	B	449/557 (80%)	0.19	30 (6%)	21	7	20, 67, 186, 230	0
2	A	313/559 (55%)	0.14	20 (6%)	23	8	27, 60, 181, 226	0
All	All	762/1116 (68%)	0.17	50 (6%)	22	7	20, 63, 182, 230	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	VAL	5.9
2	A	188	ASN	5.2
2	A	181	MET	5.1
1	B	314	LEU	4.7
2	A	398	ASP	4.6
1	B	236	HIS	4.1
1	B	237	PRO	4.1
2	A	149	SER	3.9
1	B	312	HIS	3.7
2	A	178	ILE	3.6
2	A	164	LEU	3.5
2	A	202	LEU	3.4
2	A	49	ILE	3.4
2	A	190	ALA	3.2
1	B	100	GLU	3.1
1	B	233	GLU	3.1
1	B	317	LYS	3.1
2	A	186	ILE	3.1
2	A	150	SER	3.0
1	B	316	LYS	2.8
2	A	159	ILE	2.8
1	B	245	ASN	2.8
2	A	162	THR	2.8
2	A	184	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	203	TYR	2.7
2	A	399	ALA	2.7
2	A	154	ASP	2.7
1	B	238	GLY	2.7
1	B	283	ASN	2.7
1	B	83	LEU	2.6
1	B	311	GLN	2.5
1	B	65	LEU	2.5
2	A	163	THR	2.4
1	B	228	ILE	2.4
1	B	363	LYS	2.3
2	A	478	GLY	2.3
1	B	322	VAL	2.3
1	B	290	ASP	2.3
1	B	310	ALA	2.3
1	B	332	LYS	2.3
1	B	308	GLU	2.2
1	B	361	GLU	2.2
1	B	242	ARG	2.2
1	B	241	LYS	2.2
1	B	324	ARG	2.2
1	B	328	SER	2.2
2	A	395	SER	2.2
1	B	285	LEU	2.2
2	A	397	ASN	2.1
1	B	240	PRO	2.1

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.