



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:02 AM UTC

PDB ID : 4XCI / pdb_00004xci
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)

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

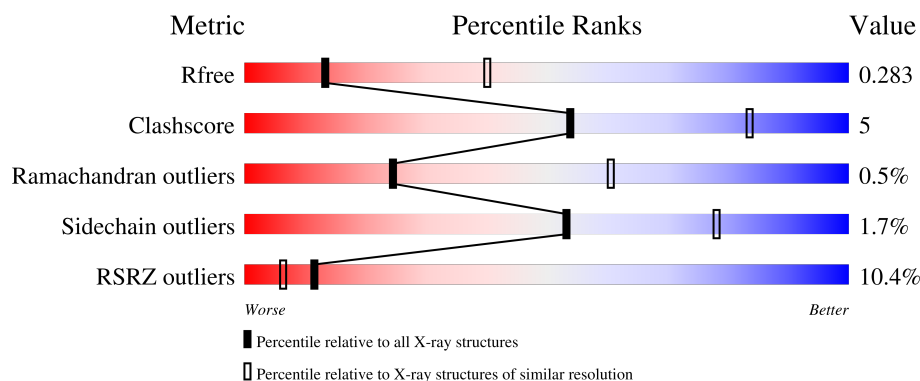
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	B	557	 7% 74% 6% 19%
2	A	559	 7% 47% 7% 44%

2 Entry composition

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.

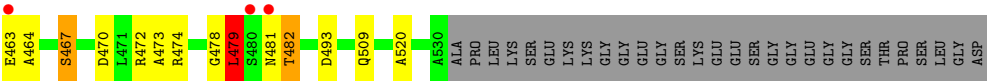
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	449	Total	C	H	N	O	S	0	0	0
			6986	2154	3577	594	651	10			

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			



4 Data and refinement statistics

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) 72.4 (41.91-3.00)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9-1692, REFMAC 5.8.0073	Depositor
R, R_{free}	0.236 , 0.266 0.255 , 0.283	Depositor DCC
R_{free} test set	1273 reflections (3.69%)	wwPDB-VP
Wilson B-factor (Å ²)	71.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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.*

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	B	0.32	0/3439	0.70	0/4636
2	A	0.36	0/2352	0.82	4/3184 (0.1%)
All	All	0.34	0/5791	0.75	4/7820 (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	A	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	191	GLU	N-CA-C	10.84	125.51	109.04
2	A	190	ALA	N-CA-C	7.49	119.45	111.28
2	A	478	GLY	N-CA-C	-7.43	104.56	115.63
2	A	479	LEU	N-CA-C	-7.41	103.22	111.82

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 ⓘ

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	35	0
All	All	5742	6031	6022	57	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 (57) 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:35:LEU:HD12	2:A:97:VAL:HG11	1.82	0.61
2:A:193:LEU:HD23	2:A:194:PRO:CD	2.31	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:462:LEU:HD22	2:A:462:LEU:C	2.32	0.54
2:A:38:SER:OG	2:A:46:LYS:NZ	2.40	0.54
2:A:159:ILE:HG21	2:A:406:ILE:HD11	1.90	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:34:MET:HE3	2:A:46:LYS:HE2	1.93	0.50
1:B:143:ILE:HD11	1:B:434:TYR:CD2	2.46	0.49
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:217:GLY:C	1:B:219:VAL:HG23	2.40	0.47
1:B:116:LEU:HB2	1:B:522:VAL:HG21	1.96	0.47
2:A:178:ILE:O	2:A:178:ILE:HG22	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:OE1	1:B:308:GLU:N	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:177:ALA:HB1	1:B:220:ASN:HB2	2.00	0.42
1:B:391:ARG:HH12	2:A:520:ALA:HB1	1.84	0.42
2:A:190:ALA:HB3	2:A:191:GLU:HG3	2.02	0.42
2:A:88:GLU:OE1	2:A:509:GLN:NE2	2.50	0.41
2:A:193:LEU:HD23	2:A:194:PRO:HD3	2.02	0.41
2:A:462:LEU:HD22	2:A:463:GLU:C	2.45	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:37:SER:HG	2:A:46:LYS:HZ1	1.67	0.40

There are no symmetry-related clashes.

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	B	437/557 (78%)	413 (94%)	23 (5%)	1 (0%)	43	76
2	A	307/559 (55%)	293 (95%)	11 (4%)	3 (1%)	12	45
All	All	744/1116 (67%)	706 (95%)	34 (5%)	4 (0%)	24	60

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 ⓘ

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%)	86	91
2	A	248/448 (55%)	239 (96%)	9 (4%)	31	65
All	All	604/897 (67%)	594 (98%)	10 (2%)	53	78

All (10) 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	411	VAL
2	A	462	LEU
2	A	467	SER

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Mol	Chain	Res	Type
2	A	479	LEU
2	A	482	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	158	ASN
1	B	245	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	B	449/557 (80%)	0.41	41 (9%) 15 8	24, 74, 199, 255	0
2	A	313/559 (55%)	0.45	38 (12%) 8 5	28, 66, 199, 255	0
All	All	762/1116 (68%)	0.43	79 (10%) 11 6	24, 70, 199, 255	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	181	MET	8.0
2	A	162	THR	6.1
1	B	178	GLY	5.9
2	A	164	LEU	5.8
1	B	249	ALA	5.1
2	A	178	ILE	5.0
2	A	481	ASN	4.8
2	A	186	ILE	4.6
2	A	163	THR	4.5
2	A	189	VAL	4.4
2	A	399	ALA	4.4
1	B	302	CYS	4.2
2	A	161	PHE	4.2
2	A	184	ASP	4.0
2	A	188	ASN	4.0
1	B	378	PRO	3.9
2	A	152	ALA	3.9
1	B	374	GLY	3.9
2	A	462	LEU	3.8
1	B	177	ALA	3.8
1	B	284	ILE	3.8
1	B	295	THR	3.7
2	A	185	ALA	3.6
2	A	193	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	218	SER	3.6
1	B	338	GLY	3.5
1	B	299	VAL	3.5
2	A	49	ILE	3.5
1	B	250	LEU	3.5
2	A	175	LEU	3.4
1	B	222	THR	3.3
2	A	182	VAL	3.3
2	A	159	ILE	3.3
2	A	183	ILE	3.3
2	A	165	ALA	3.2
1	B	175	ALA	3.1
1	B	203	TYR	3.0
1	B	357	ALA	3.0
1	B	322	VAL	3.0
1	B	243	ILE	3.0
2	A	398	ASP	3.0
1	B	314	LEU	2.9
1	B	216	GLY	2.9
1	B	248	ILE	2.9
1	B	292	ILE	2.9
2	A	480	SER	2.9
2	A	147	LEU	2.8
2	A	395	SER	2.8
1	B	240	PRO	2.8
2	A	157	ARG	2.8
1	B	300	VAL	2.8
1	B	83	LEU	2.8
2	A	463	GLU	2.7
2	A	187	VAL	2.7
1	B	356	ALA	2.7
1	B	533	ALA	2.6
2	A	156	LEU	2.5
1	B	220	ASN	2.5
2	A	202	LEU	2.4
1	B	337	THR	2.4
1	B	104	ASP	2.3
1	B	391	ARG	2.3
2	A	144	ILE	2.3
1	B	317	LYS	2.3
1	B	372	VAL	2.3
1	B	223	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	324	ARG	2.3
2	A	194	PRO	2.2
2	A	190	ALA	2.2
1	B	320	LEU	2.2
1	B	285	LEU	2.2
1	B	101	GLU	2.2
1	B	158	ASN	2.2
1	B	376	LYS	2.1
2	A	396	ILE	2.1
2	A	151	VAL	2.1
1	B	246	ALA	2.1
2	A	410	PRO	2.1
2	A	195	ASN	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.