wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:26 PM GMT

PDB ID	:	1TMH
Title	:	MODULAR MUTAGENESIS OF A TIM-BARREL ENZYME: THE CRYSTAL STRUCTURE OF A CHIMERIC E. COLI TIM HAVING THE EIGHTH (BETA-ALPHA)-UNIT REPLACED BY THE EQUIVALENT UNIT OF CHICKEN TIM
Authors	:	Radha Kishan, K.V.; Zeelen, J.Ph.; Wierenga, R.K.
Deposited on	:	1994-03-22
Resolution	:	2.80 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 (i) symbol.

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

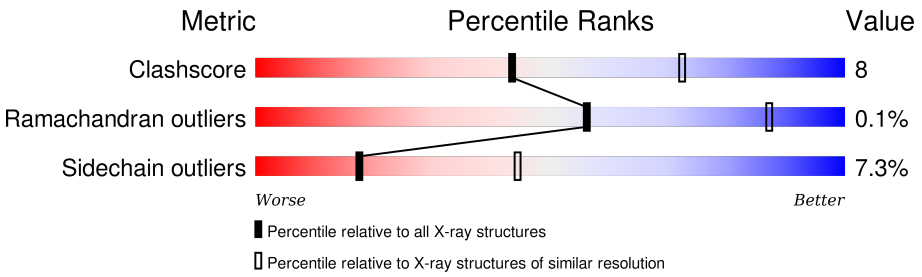
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	254	72% 22% 6%
1	B	254	72% 24% •
1	C	254	73% 21% 6%
1	D	254	71% 23% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7628 atoms, of which 4 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 TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	254	1902	1193	1	334	364	10	0	0	0
1	B	254	1902	1193	1	334	364	10	0	0	0
1	C	254	1902	1193	1	334	364	10	0	0	0
1	D	254	1902	1193	1	334	364	10	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	HIS	PRO	ENGINEERED	UNP P0A858
A	229	VAL	ILE	ENGINEERED	UNP P0A858
A	232	PHE	ALA	ENGINEERED	UNP P0A858
A	241	PRO	ALA	ENGINEERED	UNP P0A858
A	?	-	ASP	DELETION	UNP P0A858
A	243	GLU	ALA	ENGINEERED	UNP P0A858
A	245	VAL	ALA	ENGINEERED	UNP P0A858
A	246	ASP	VAL	ENGINEERED	UNP P0A858
A	248	ILE	VAL	ENGINEERED	UNP P0A858
A	249	ASN	LYS	ENGINEERED	UNP P0A858
B	227	HIS	PRO	ENGINEERED	UNP P0A858
B	229	VAL	ILE	ENGINEERED	UNP P0A858
B	232	PHE	ALA	ENGINEERED	UNP P0A858
B	241	PRO	ALA	ENGINEERED	UNP P0A858
B	?	-	ASP	DELETION	UNP P0A858
B	243	GLU	ALA	ENGINEERED	UNP P0A858
B	245	VAL	ALA	ENGINEERED	UNP P0A858
B	246	ASP	VAL	ENGINEERED	UNP P0A858
B	248	ILE	VAL	ENGINEERED	UNP P0A858
B	249	ASN	LYS	ENGINEERED	UNP P0A858
C	227	HIS	PRO	ENGINEERED	UNP P0A858

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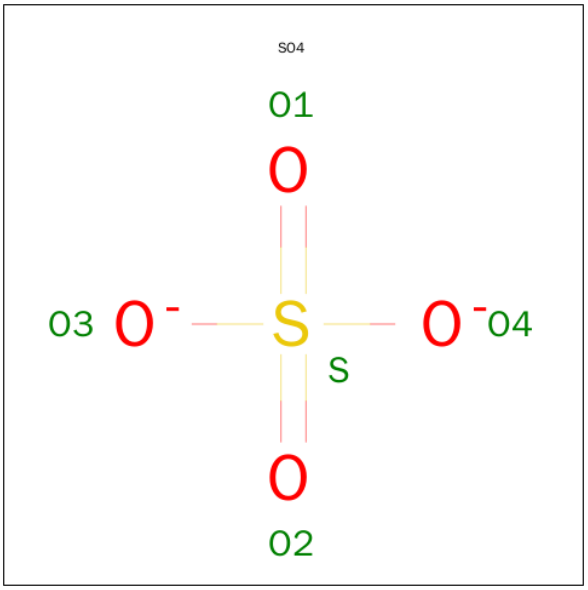
Chain	Residue	Modelled	Actual	Comment	Reference
C	229	VAL	ILE	ENGINEERED	UNP P0A858
C	232	PHE	ALA	ENGINEERED	UNP P0A858
C	241	PRO	ALA	ENGINEERED	UNP P0A858
C	?	-	ASP	DELETION	UNP P0A858
C	243	GLU	ALA	ENGINEERED	UNP P0A858
C	245	VAL	ALA	ENGINEERED	UNP P0A858
C	246	ASP	VAL	ENGINEERED	UNP P0A858
C	248	ILE	VAL	ENGINEERED	UNP P0A858
C	249	ASN	LYS	ENGINEERED	UNP P0A858
D	227	HIS	PRO	ENGINEERED	UNP P0A858
D	229	VAL	ILE	ENGINEERED	UNP P0A858
D	232	PHE	ALA	ENGINEERED	UNP P0A858
D	241	PRO	ALA	ENGINEERED	UNP P0A858
D	?	-	ASP	DELETION	UNP P0A858
D	243	GLU	ALA	ENGINEERED	UNP P0A858
D	245	VAL	ALA	ENGINEERED	UNP P0A858
D	246	ASP	VAL	ENGINEERED	UNP P0A858
D	248	ILE	VAL	ENGINEERED	UNP P0A858
D	249	ASN	LYS	ENGINEERED	UNP P0A858

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0

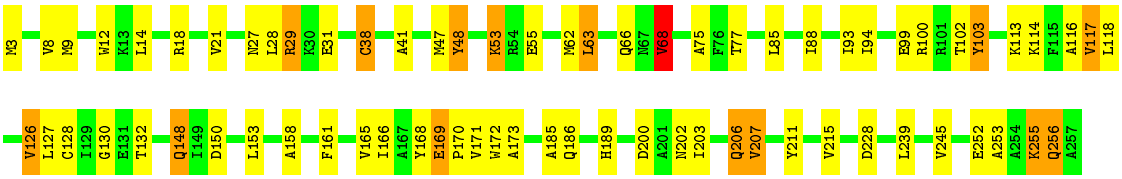
3 Residue-property plots (i)

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.

Note EDS was not executed.

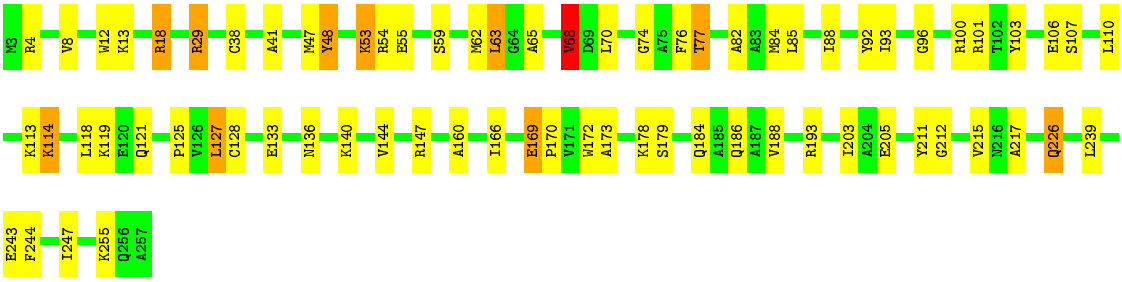
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A: 72% 22% 6%



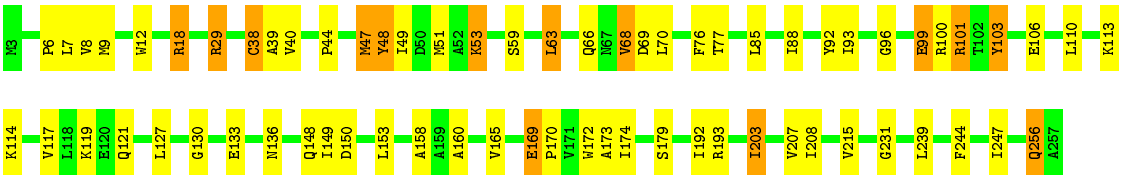
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B: 72% 24% •



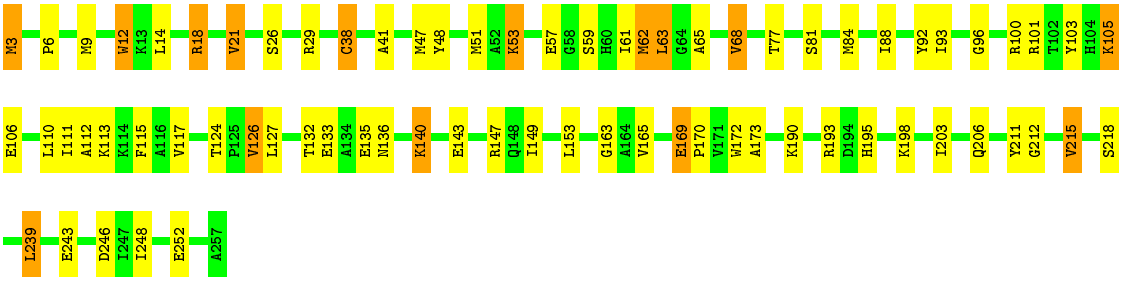
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain C: 73% 21% 6%



- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain D: 71% 23% 6%


M3
P6
M9
W12
K13
L14
R18
V21
S26
R29
C38
A41
M47
Y48
M51
A52
K53
E57
G58
S59
H60
I61
M62
L63
G64
A65
V68
T77
S81
H84
I88
Y92
I93
G96
R100
R101
T102
Y103
H104
K105
E106
L110
I111
A112
K113
K114
F115
A116
V117
T124
P125
V126
L127
T132
E133
A134
E135
N136
K140
E143
R147
Q148
I149
L153
G163
A164
V165
E169
P170
V171
W172
A173
K190
R193
D194
H195
K198
I203
Q206
Y211
G212
V215
S218
L239
E243
D246
I247
I248
E252
A257

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.64Å 118.31Å 58.98Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	35.10 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (35.10-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7628	wwPDB-VP
Average B, all atoms ($Å^2$)	18.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.96	0/1932	1.63	28/2612 (1.1%)
1	B	0.96	0/1932	1.60	25/2612 (1.0%)
1	C	0.96	0/1932	1.61	24/2612 (0.9%)
1	D	0.94	0/1932	1.58	27/2612 (1.0%)
All	All	0.95	0/7728	1.60	104/10448 (1.0%)

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
1	A	0	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	A	29	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	A	103	TYR	CB-CG-CD2	-9.77	115.14	121.00
1	A	18	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	D	103	TYR	CB-CG-CD2	-9.36	115.38	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	TYR	Sidechain
1	A	211	TYR	Sidechain
1	D	211	TYR	Sidechain

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	A	1901	1	1892	35	0
1	B	1901	1	1892	36	0
1	C	1901	1	1892	31	0
1	D	1901	1	1892	33	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
All	All	7624	4	7568	123	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 8.

The worst 5 of 123 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:D:65:ALA:HB3	1:D:93:ILE:HD12	1.70	0.74
1:A:53:LYS:HE3	1:B:18:ARG:HH22	1.55	0.72
1:C:169:GLU:HB2	1:C:174:ILE:HD11	1.76	0.67
1:A:8:VAL:HG23	1:A:38:CYS:SG	2.35	0.67
1:C:8:VAL:HG23	1:C:38:CYS:SG	2.35	0.66

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	252/254 (99%)	238 (94%)	14 (6%)	0	100	100
1	B	252/254 (99%)	234 (93%)	18 (7%)	0	100	100
1	C	252/254 (99%)	240 (95%)	12 (5%)	0	100	100
1	D	252/254 (99%)	236 (94%)	15 (6%)	1 (0%)	39	74
All	All	1008/1016 (99%)	948 (94%)	59 (6%)	1 (0%)	56	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	105	LYS

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	191/191 (100%)	177 (93%)	14 (7%)	17	44
1	B	191/191 (100%)	178 (93%)	13 (7%)	20	49
1	C	191/191 (100%)	176 (92%)	15 (8%)	15	40
1	D	191/191 (100%)	177 (93%)	14 (7%)	17	44
All	All	764/764 (100%)	708 (93%)	56 (7%)	17	44

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	239	LEU
1	C	63	LEU
1	D	203	ILE
1	B	255	LYS
1	C	44	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	GLN
1	B	210	GLN
1	C	210	GLN
1	B	91	GLN
1	C	148	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	555	-	4,4,4	1.12	0	6,6,6	0.20	0
2	SO4	B	556	-	4,4,4	0.86	0	6,6,6	0.35	0
2	SO4	C	557	-	4,4,4	0.69	0	6,6,6	0.22	0
2	SO4	D	558	-	4,4,4	1.22	0	6,6,6	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	555	-	-	0/0/0/0	0/0/0/0
2	SO4	B	556	-	-	0/0/0/0	0/0/0/0
2	SO4	C	557	-	-	0/0/0/0	0/0/0/0
2	SO4	D	558	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.