

EDS summary for PDB entry 2xse.

The following statistics were obtained using the structure factors deposited for your PDB entry, using a customised version of the Uppsala Electron Density Server (EDS) running at PDBe. More information about EDS and the output presented here can be found on the original EDS site (<http://eds.bmc.uu.se>).

Resolution	
Resolution from map-calculations (low)	36.45Å
Resolution from map-calculations (high)	1.90Å
Resolution from PDB header	1.90Å
R-factors	
R-factor for map	0.198
R-factor from PDB header	0.176
Free R-factor from PDB header	0.200
Structure quality	
Average Real space R-factor (Deviation)	0.150 (0.100)
Average Real-space correlation coefficient (Deviation)	0.917 (0.083)
Average Occupancy-weighted avg temperature factor (Deviation)	44.8Å ² (19.1Å ²)
Padilla-Yeates statistics	
Padilla-Yeates < L >	0.471
Padilla-Yeates <L ² >	0.297
Wilson statistics	
Wilson B-factor	28.3 Å ²
Wilson Scale	0.769
Wilson Omega	1.398
Crystal data	
Space group	P 61 2 2
Total no. of reflections	20595
Number of reflections used	20595
Completeness of data	99.8%

PQS summary for PDB entry 2xse.

Assemblies are generated using the Protein Quaternary Structure server (PQS). PQS uses crystal symmetry matrices to generate symmetry-related copies of the chains in a PDB entry and, by considering the buried surface area between pairs of chains, determines the likelihood of that contact being of some biological significance. The algorithm is described in the PQS documentation on the PDBe website.

Biomolecule 1: Monomeric

Chain A is monomeric, therefore no assembly statistics available.

Sequence-matching information for PDB entry 2xse.

We have matched your sequence for chain/s: A ... to the following UniProt Reference and alignment. Please comment if this is correct. UniProt represents the combined TREMBL, SWISSPROT and PIR sequence databases. More information about UniProt may be found at the Uniprot website (<http://www.uniprot.org>).

INFORMATION FOR CHAIN A

UNP ACCESSION NUMBER: Q9U6M1

UNP ORGANISM SCIENTIFIC: LEISHMANIA TARENTOLAE

TAX ID: 5689

UNP SEQUENCE START-END POSITION(S): 392 - 561

UNP-PDB ATOM RECORDS ALIGNMENT:

UNP	1	MEPDSKKVKLDIFNFPTTRETRTPPEVAESYAEAVKSHPFYDNVHSVVD	50
PDB	1	-----	0
UNP	51	YDSGTIKDGRGQIIGVVLREALPKYAASMASELLTSAAVRTSLRSMFGG	100
PDB	1	-----	0
UNP	101	EPPLSGIAGYFDYRGSVELKSRKTSFTYEHEAAWPAVFPVVDYVSEIYR	150
PDB	1	-----	0
UNP	151	HVAPERWKAQNDAIPDLVRIHGTFFSTLTINSRFRASHTDVGDFDAGYS	200
PDB	1	-----	0
UNP	201	CIACLDGQFKGLALSFDDFGINVLLQPRDVMIFDSHHFHSNTEVELSFSG	250
PDB	1	-----	0
UNP	251	EDWKRLTCVFYRAALGEPASYAEYQRRLEKSKTDTRFTPVVHHVRVKEN	300
PDB	1	-----	0
UNP	301	GTSVNRPSVPYISQSPFWVPMVAHCLQHCASAAQCVHEAMTADGSRLAE	350
PDB	1	-----	0
UNP	351	MMFGESLSTSDGIPLRGEDEVKANGDSTPRPLSRLGGFSETNLMVSTAV	400
PDB	1	-----T N L M V S T A V	9
UNP	401	EKKKYLDSEFLLHCISAQLLDMWKQARARWLELVGKEWAHMLALNPERKD	450
PDB	10	EKKKYLDSEFLLHCISAQLLDMWKQARARWLELVGKEWAHMLALNPERKD	59
UNP	451	FLWKNQSEMNSAFFDLCEVGKQVMLGLLGKEVALPKEEQAFWIMYAVHLS	500
PDB	60	FLWKNQSEMNSAFFDLCEVGKQVMLGLLGKEVALPKEEQAFWIMYAVHLS	109
UNP	501	AACAEELHMPEVAMSLRKLNVKLDKDFNFGGTRYFKDMPPEEKRRMERKQ	550
PDB	110	AACAEELHMPEVAMSLRKLNVKLDKDFNFGGTRYFKDMPPEEKRRMERKQ	159
UNP	551	RIEEARRHGMPSGSHEKRANWLTNDSFDYQTEDCVIDYAQHKWVLPALHA	600
PDB	160	RIEEARRHGMP-----	170
UNP	601	KEVTKTVRTGELPTTERVVRVLVVI PDPQSKLENDCKLEVDPDMVGSSE	650
PDB	171	-----	170
UNP	651	WERLMSSPAVHRVLSAAQRNLQLPDSVTHGNVQTHFAFHSTLPTDIYDFV	700
PDB	171	-----	170
UNP	701	VLQHVLSRIPDDAQASAYIRRAALCSGCLFVVETDVQCROYITLKY SIR	750
PDB	171	-----	170
UNP	751	CSYDTPVAPLFFQQLHRVCYGTKTARVRTKGELES LIPTVCCARYKLGSP	800
PDB	171	-----	170

UNP
PDB

801 LNTTVHVVSPPFPSCEVQNLSSALCDRA
171 -----

827
170

CONFIDENTIAL: VALIDATION REPORT

Deviations from expected geometric properties (REMARK 500) for PDB entry 2xse.

REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: TORSION ANGLES
REMARK 500
REMARK 500 TORSION ANGLES OUTSIDE THE EXPECTED RAMACHANDRAN REGIONS:
REMARK 500 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER;
REMARK 500 SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,4X,F7.2,3X,F7.2)
REMARK 500
REMARK 500 EXPECTED VALUES: GJ KLEYWEGT AND TA JONES (1996). PHI/PSI-
REMARK 500 CHOLOGY: RAMACHANDRAN REVISITED. STRUCTURE 4, 1395 - 1400
REMARK 500
REMARK 500 M RES CSSEQI PSI PHI
REMARK 500 LYS A 402 4.68 -69.68
REMARK 500 HIS A 413 -5.88 75.65
REMARK 500 MSE A 514 78.69 -105.40
REMARK 500
REMARK 500 REMARK: NULL