EDS summary for PDB entry 4tst.

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)	24.74Å
Resolution from map-calculations (high)	2.50Å
Resolution from PDB header	2.50Å

R-factors

R-factor for map	0.279
R-factor from PDB header	0.164
Free R-factor from PDB header	0.216

Structure quality

Average Real space R-factor (Deviation)	0.214 (0.115)
Average Real-space correlation coefficient (Deviation)	0.872 (0.144)
Average Occupancy-weighted avg temperature factor (Deviation)	44.1Å^2 (16.8Å^2)

Padilla-Yeates statistics

Padilla-Yeates <|L|>	0.488
Padilla-Yeates <L^2>	0.318

Wilson statistics

Wilson B-factor	56.7 Å^2
Wilson Scale	0.574
Wilson Omega	1.681

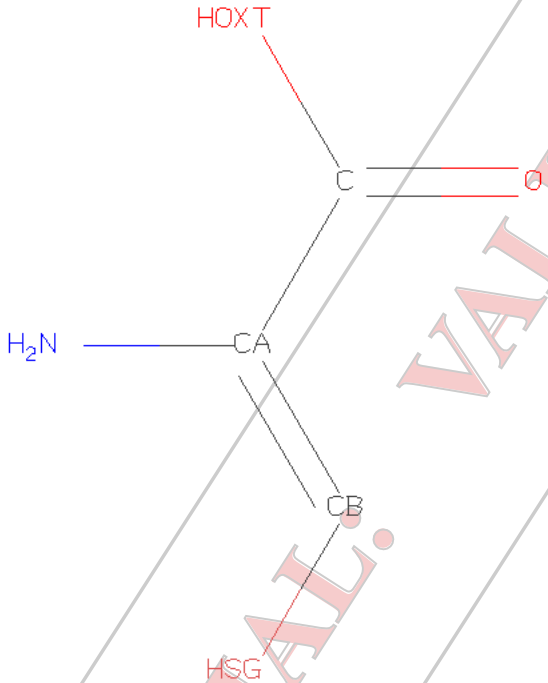
Crystal data

Space group	P 21 21 21
Total no. of reflections	14096
Number of reflections used	14096
Completeness of data	98.9%

Heterogen summary for PDB entry 4tst.

The following heterogenic group is new to the PDB. We have created a dictionary description for the molecule as shown below. Please comment on whether the details given here are correct.

Heterogen code:	BB9
Systematic name:	"(2Z)-2-amino-3-sulfanylprop-2-enoic acid"
Deposition date:	No date available
Release status:	
Formula:	C3 H5 N O2 S (119.1 Da)
Polymer type:	"L-PEPTIDE-LINKING"
SMILES string:	NC(=CS)C(O)=O
Stereo SMILES string:	N\C(=C/S)C(O)=O
InChi string:	1/C3H5NO2S/c4-2(1-7)3(5)6/h1,7H,4H2,(H,5,6)/b2-1-/f/h5H



Atom-1	*Atom-2*	*Bond-order*
N	CA	SING
CA	C	SING
CA	CB	DOUB
C	O	DOUB
C	OXT	SING
CB	SG	SING
N	HN1	SING
N	HN2	SING
CB	HB	SING

OXT	HXT	SING
SG	HG	SING

PQS summary for PDB entry 4tst.

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:

Accessible surface areas	Isolated chain A (2 copies):	17149.2Å^2
	Total area of all isolated chains:	32175.4Å^2
	Total buried surface area of assembly:	1061.5Å^2
Solvation free energies	Isolated chain A:	-314.3 kcal/mol
	Total energy for complete complex:	-646.0 kcal/mol
	Energy gain upon complex formation:	-17.5 kcal/mol
Salt bridges	Number formed in assembly:	0

Sequence-matching information for PDB entry 4tst.

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: P10153
UNP ORGANISM SCIENTIFIC: HOMO SAPIENS
TAX ID: 9606
PFAM ACCESSION NUMBER(S): PF00074
INTERPRO ACCESSION NUMBER(S): IPR001427
UNP SEQUENCE START-END POSITION(S): 27 - 161
UNP-PDB ATOM RECORDS ALIGNMENT:

```
UNP                1 MVPKLFTSQICLLLLLGLLAVEGSLHVKPPQFTWAQWFETQHINMTSQQC     50
                                                :|||||||||||||||||||||||
PDB                1 -------------------------MKPPQFTWAQWFETQHINMTSQQC     24

UNP               51 TNAMQVINNYQRRCKNQNTFLLTTFANVVNVCGNPNMTCPSNKTRKNCHH    100
                     ||||||||||||||||||||||||||||||||||||||||||||||||||
PDB               25 TNAMQVINNYQRRCKNQNTFLLTTFANVVNVCGNPNMTCPSNKTRKNCHH     74

UNP              101 SGSQVPLIHCNLTTPSPQNISNCRYAQTPANMFYIVACDNRDQRRDPPQY    150
                     ||||||||||||||||||||||||||||||||||||||||||||||||||
PDB               75 SGSQVPLIHCNLTTPSPQNISNCRYAQTPANMFYIVACDNRDQRRDPPQY    124

UNP              151 PVVPVHLDRII    161
                     ||||||||||||
PDB              125 PVVPVHLDRII    135
```

Deviations from expected geometric properties (REMARK 500) for PDB entry 4tst.

```
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS
REMARK 500
REMARK 500 THE FOLLOWING ATOMS THAT ARE RELATED BY CRYSTALLOGRAPHIC
REMARK 500 SYMMETRY ARE IN CLOSE CONTACT.  AN ATOM LOCATED WITHIN 0.15
REMARK 500 ANGSTROMS OF A SYMMETRY RELATED ATOM IS ASSUMED TO BE ON A
REMARK 500 SPECIAL POSITION AND IS, THEREFORE, LISTED IN REMARK 375
REMARK 500 INSTEAD OF REMARK 500.  ATOMS WITH NON-BLANK ALTERNATE
REMARK 500 LOCATION INDICATORS ARE NOT INCLUDED IN THE CALCULATIONS.
REMARK 500
REMARK 500 DISTANCE CUTOFF:
REMARK 500 2.2 ANGSTROMS FOR CONTACTS NOT INVOLVING HYDROGEN ATOMS
REMARK 500 1.6 ANGSTROMS FOR CONTACTS INVOLVING HYDROGEN ATOMS
REMARK 500
REMARK 500  ATM1  RES C  SSEQI   ATM2  RES C  SSEQI  SSYMOP   DISTANCE
REMARK 500   O    HOH A  2003     O    HOH A  2066     5545     1.72
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES PROTEIN: ENGH AND HUBER, 1999
REMARK 500 EXPECTED VALUES NUCLEIC ACID: CLOWNEY ET AL 1996
REMARK 500
REMARK 500  M RES CSSEQI ATM1   ATM2   ATM3
REMARK 500    ASP A  43   CB  -  CG  -  OD1 ANGL. DEV. =   7.5 DEGREES
REMARK 500    ASP A 126   CB  -  CG  -  OD1 ANGL. DEV. =   6.5 DEGREES
REMARK 500    ASP A 235   CB  -  CG  -  OD1 ANGL. DEV. =   7.1 DEGREES
REMARK 500    LEU A 335   CB  -  CG  -  CD1 ANGL. DEV. = -10.4 DEGREES
REMARK 500    LEU A 335   CB  -  CG  -  CD2 ANGL. DEV. =  12.1 DEGREES
REMARK 500    ARG A 337   NE  -  CZ  -  NH1 ANGL. DEV. =   3.5 DEGREES
REMARK 500    ARG A 337   NE  -  CZ  -  NH2 ANGL. DEV. =  -5.0 DEGREES
REMARK 500
REMARK 500 REMARK: NULL
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    LEU A 140      118.22    -38.91
REMARK 500    ASP A 253       19.91     56.20
REMARK 500    ASN A 254       84.11   -150.03
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
```

```
REMARK 500 SUBTOPIC: NON-CIS, NON-TRANS
REMARK 500
REMARK 500 THE FOLLOWING PEPTIDE BONDS DEVIATE SIGNIFICANTLY FROM BOTH
REMARK 500 CIS AND TRANS CONFORMATION.  CIS BONDS, IF ANY, ARE LISTED
REMARK 500 ON CISPEP RECORDS.  TRANS IS DEFINED AS 180 +/- 30 AND
REMARK 500 CIS IS DEFINED AS 0 +/- 30 DEGREES.
REMARK 500                                    MODEL     OMEGA
REMARK 500 ASP A  253     ASN A  254                    149.45
REMARK 500
REMARK 500 REMARK: NULL
```