

wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 - 08:10 AM EDT

PDB ID	:	1DST
Title	:	MUTANT OF FACTOR D WITH ENHANCED CATALYTIC ACTIVITY
Authors	:	Narayana, S.V.L.; Volanakis, J.E.
Deposited on	:	1995-09-13
Resolution	:	2.00 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

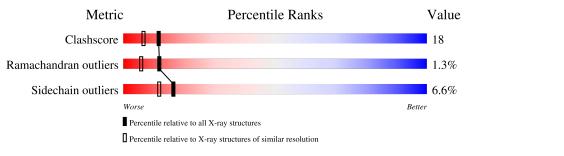
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.00 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	$egin{array}{llllllllllllllllllllllllllllllllllll$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
Clashscore	141614	9178 (2.00-2.00)		
Ramachandran outliers	138981	9054 (2.00-2.00)		
Sidechain outliers	138945	9053 (2.00-2.00)		

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 <=5%

Mol	Chain	Length	Quality of chain					
1	А	228	72%	21%	5%•			



1DST

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1786 atoms, of which 0 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 FACTOR D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	228	Total 1725	C 1071	N 326	0 318	S 10	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	94	TYR	SER	engineered mutation	UNP P00746
А	214	SER	THR	engineered mutation	UNP P00746
А	215	TRP	SER	engineered mutation	UNP P00746

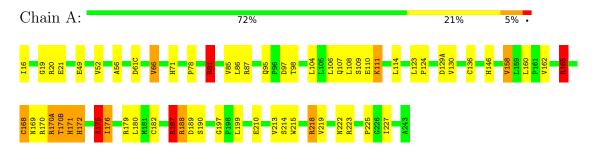
• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	61	Total O 61 61	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: FACTOR D



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	45.38Å 45.38Å 175.21Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.50 - 2.00	Depositor
Resolution (A)	9.99 - 2.00	EDS
% Data completeness	(Not available) $(7.50-2.00)$	Depositor
(in resolution range)	88.4 (9.99-2.00)	EDS
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available), 0.213	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.259 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	15.6	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.43 , 74.4	EDS
L-test for twinning ¹	$< L >=0.45, < L^2>=0.27$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	1786	wwPDB-VP
Average B, all atoms $(Å^2)$	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.39% of the height of the origin peak. No significant pseudotranslation is detected.

¹Theoretical 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 (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	Bo	nd lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.73	3/1763~(0.2%)	1.06	12/2400~(0.5%)	

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	А	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	171	HIS	C-N	-7.79	1.16	1.34
1	А	175	ALA	C-N	6.46	1.49	1.34
1	А	182	CYS	CB-SG	5.43	1.91	1.82

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	176	ILE	CA-CB-CG1	10.10	130.18	111.00
1	А	170(A)	ARG	NE-CZ-NH2	7.51	124.05	120.30
1	А	170	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	А	223	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	А	188	ARG	NE-CZ-NH2	7.11	123.86	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group		
1	А	165	ARG	Sidechain		
1	А	175	ALA	Mainchain		

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Mol	Chain	Res	Type	Group
1	А	188	ARG	Sidechain
1	А	20	ARG	Sidechain
1	А	81	ARG	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	А	1725	0	1701	60	0
2	А	61	0	0	3	0
All	All	1786	0	1701	60	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 18.

The worst 5 of 60 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:A:168:CYS:SG	1:A:176:ILE:HD13	1.79	1.22
1:A:187:ARG:HH11	1:A:187:ARG:HG3	1.24	0.99
1:A:187:ARG:HH11	1:A:187:ARG:CG	1.87	0.88
1:A:168:CYS:SG	1:A:176:ILE:CD1	2.63	0.86
1:A:170(A):ARG:CZ	1:A:225:PRO:HG3	2.06	0.86

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	А	226/228~(99%)	213~(94%)	10 (4%)	3~(1%)	12 6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	175	ALA
1	А	170(B)	THR
1	А	172	HIS

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	А	182/182~(100%)	170~(93%)	12~(7%)	16 12

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	160	LEU
1	А	162	VAL
1	А	218	ARG
1	А	165	ARG
1	А	108	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such side chains are listed below:

Mol	Chain	Res	Type
1	А	71	HIS
1	А	75	GLN
1	А	146	HIS
1	А	107	GLN
1	А	65	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 monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	А	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	171:HIS	С	172:HIS	Ν	1.16



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

