



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:25 pm BST

PDB ID : 1SCA
Title : ENZYME CRYSTAL STRUCTURE IN A NEAT ORGANIC SOLVENT
Authors : Fitzpatrick, P.A.; Steinmetz, A.C.U.; Ringe, D.; Klibanov, A.M.
Deposited on : 1993-07-19
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

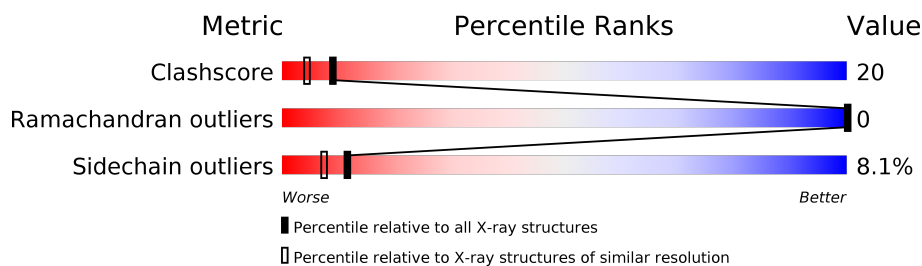
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	274	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2050 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 SUBTILISIN CARLSBERG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	1	0
			1921	1190	332	394	5			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	SER	THR	CONFLICT	UNP P00780
A	129	ALA	PRO	CONFLICT	UNP P00780
A	158	ASN	SER	CONFLICT	UNP P00780
A	161	SER	ASN	CONFLICT	UNP P00780
A	212	ASN	SER	CONFLICT	UNP P00780

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

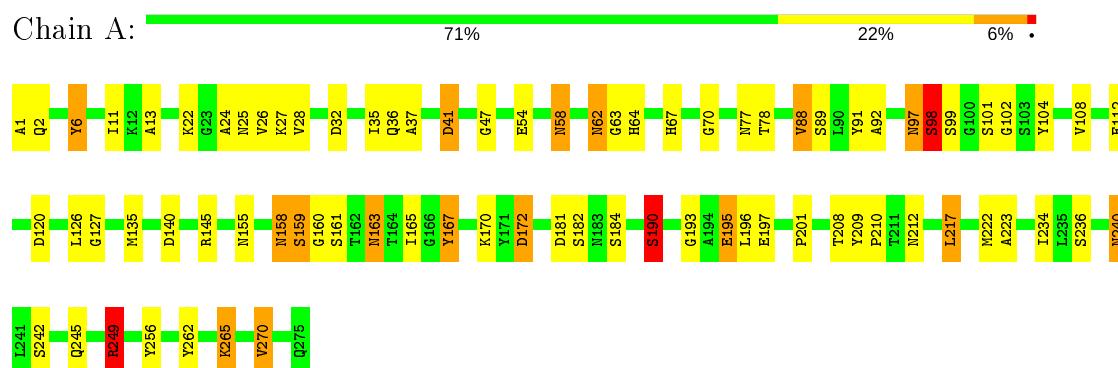
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total	O	0	0
			126	126		

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 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.

Note EDS was not executed.

• Molecule 1: SUBTILISIN CARLSBERG



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.50 Å 55.30 Å 53.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.156 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2050	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: NA, CA

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	1.17	8/1958 (0.4%)	1.57	31/2670 (1.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190[A]	SER	CB-OG	-23.92	1.11	1.42
1	A	190[B]	SER	CB-OG	-23.92	1.11	1.42
1	A	91	TYR	CD1-CE1	9.20	1.53	1.39
1	A	195	GLU	CD-OE2	6.09	1.32	1.25
1	A	91	TYR	CE1-CZ	-5.53	1.31	1.38
1	A	197	GLU	CD-OE1	5.35	1.31	1.25
1	A	112	GLU	CD-OE2	5.35	1.31	1.25
1	A	54	GLU	CD-OE1	5.27	1.31	1.25

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASP	CB-CG-OD1	10.94	128.15	118.30
1	A	120	ASP	CB-CG-OD1	-10.24	109.09	118.30
1	A	181	ASP	CB-CG-OD2	-9.68	109.59	118.30
1	A	140	ASP	CB-CG-OD1	8.73	126.16	118.30
1	A	167	TYR	CB-CG-CD1	-8.40	115.96	121.00
1	A	41	ASP	CB-CG-OD1	7.95	125.45	118.30
1	A	249	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	172	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	140	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	91	TYR	CG-CD1-CE1	-6.63	115.99	121.30
1	A	91	TYR	CZ-CE2-CD2	-6.49	113.96	119.80
1	A	270	VAL	CG1-CB-CG2	-6.38	100.69	110.90
1	A	145	ARG	NE-CZ-NH1	6.32	123.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	A	159	SER	C-N-CA	-5.95	109.81	122.30
1	A	1	ALA	N-CA-CB	5.86	118.30	110.10
1	A	32	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	A	249	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	1	ALA	CB-CA-C	5.49	118.33	110.10
1	A	120	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	88	VAL	CG1-CB-CG2	-5.36	102.32	110.90
1	A	236	SER	N-CA-CB	5.25	118.38	110.50
1	A	91	TYR	CD1-CG-CD2	5.25	123.67	117.90
1	A	6	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	A	262	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	A	98	SER	N-CA-CB	-5.21	102.68	110.50
1	A	6	TYR	CB-CG-CD2	5.19	124.11	121.00
1	A	184	SER	N-CA-CB	5.14	118.21	110.50
1	A	37	ALA	CB-CA-C	5.07	117.71	110.10
1	A	91	TYR	CE1-CZ-CE2	5.04	127.87	119.80
1	A	91	TYR	CB-CG-CD1	-5.01	118.00	121.00

There are no chirality outliers.

There are no planarity outliers.

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	A	1921	0	1881	77	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	126	0	0	10	0
All	All	2050	0	1881	77	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 20.

All (77) 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:242:SER:H	1:A:245:GLN:NE2	1.47	1.11
1:A:242:SER:N	1:A:245:GLN:HE21	1.54	1.06
1:A:2:GLN:HE22	1:A:77:ASN:H	1.06	0.97
1:A:163:ASN:ND2	1:A:165:ILE:H	1.67	0.93
1:A:36:GLN:HE22	1:A:212:ASN:H	1.20	0.89
1:A:62:ASN:HD22	1:A:64:HIS:H	1.24	0.84
1:A:249:ARG:NH1	4:A:903:HOH:O	2.08	0.84
1:A:26:VAL:O	1:A:88:VAL:HG23	1.77	0.83
1:A:28:VAL:HG23	1:A:88:VAL:HG21	1.62	0.81
1:A:2:GLN:NE2	1:A:77:ASN:H	1.82	0.74
1:A:172:ASP:HB2	4:A:902:HOH:O	1.90	0.72
1:A:158:ASN:HD22	1:A:158:ASN:H	1.35	0.72
1:A:155:ASN:ND2	4:A:800:HOH:O	1.87	0.72
1:A:97:ASN:ND2	1:A:101:SER:H	1.90	0.69
1:A:25:ASN:OD1	4:A:667:HOH:O	2.10	0.69
1:A:158:ASN:N	1:A:158:ASN:HD22	1.90	0.69
1:A:242:SER:N	1:A:245:GLN:NE2	2.27	0.67
1:A:165:ILE:HD12	1:A:193:GLY:HA3	1.79	0.64
1:A:163:ASN:ND2	1:A:165:ILE:N	2.45	0.61
1:A:2:GLN:HE22	1:A:77:ASN:N	1.89	0.60
1:A:97:ASN:HD22	1:A:97:ASN:C	2.05	0.60
1:A:104:TYR:HD1	1:A:135:MET:CE	2.16	0.59
1:A:240:ASN:HB3	4:A:525:HOH:O	2.02	0.59
1:A:158:ASN:H	1:A:158:ASN:ND2	2.01	0.58
1:A:163:ASN:HD22	1:A:163:ASN:C	2.07	0.57
1:A:163:ASN:OD1	1:A:195:GLU:OE1	2.22	0.57
1:A:58:ASN:H	1:A:58:ASN:HD22	1.51	0.57
1:A:28:VAL:CG2	1:A:88:VAL:HG21	2.33	0.56
1:A:159:SER:O	1:A:160:GLY:C	2.43	0.56
1:A:63:GLY:HA2	1:A:210:PRO:CG	2.37	0.55
1:A:62:ASN:ND2	1:A:64:HIS:H	2.00	0.54
1:A:102:GLY:HA2	4:A:905:HOH:O	2.07	0.53
1:A:158:ASN:N	1:A:158:ASN:ND2	2.57	0.53
1:A:170:LYS:NZ	4:A:856:HOH:O	2.41	0.52
1:A:13:ALA:HA	1:A:270:VAL:HG21	1.91	0.52
1:A:6:TYR:CE1	1:A:182:SER:HA	2.44	0.52
1:A:27:LYS:NZ	4:A:574:HOH:O	2.37	0.51
1:A:97:ASN:HD21	1:A:101:SER:H	1.59	0.51
1:A:58:ASN:ND2	1:A:58:ASN:H	2.08	0.51
1:A:242:SER:H	1:A:245:GLN:HE21	0.68	0.50
1:A:209:TYR:CG	1:A:210:PRO:HD2	2.46	0.50
1:A:88:VAL:HG22	1:A:89:SER:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:HD12	1:A:193:GLY:CA	2.43	0.49
1:A:11:ILE:O	1:A:270:VAL:HG22	2.12	0.49
1:A:58:ASN:N	1:A:58:ASN:HD22	2.08	0.49
1:A:127:GLY:HA2	1:A:167:TYR:O	2.13	0.49
1:A:163:ASN:C	1:A:163:ASN:ND2	2.66	0.48
1:A:25:ASN:HA	4:A:667:HOH:O	2.12	0.48
1:A:36:GLN:HE21	1:A:210:PRO:HA	1.80	0.47
1:A:35:ILE:HD12	1:A:92:ALA:HB2	1.97	0.47
1:A:163:ASN:HD21	1:A:165:ILE:H	1.57	0.47
1:A:63:GLY:HA2	1:A:210:PRO:HG3	1.97	0.47
1:A:201:PRO:O	1:A:223:ALA:HA	2.16	0.46
1:A:209:TYR:CD1	1:A:210:PRO:HD2	2.51	0.46
1:A:108:VAL:HG22	1:A:135:MET:HA	1.97	0.46
1:A:163:ASN:HD21	1:A:165:ILE:HB	1.81	0.45
1:A:24:ALA:O	1:A:25:ASN:HB3	2.15	0.45
1:A:126:LEU:C	1:A:126:LEU:HD12	2.37	0.45
1:A:165:ILE:HD11	1:A:196:LEU:HB2	2.00	0.44
1:A:240:ASN:H	1:A:240:ASN:ND2	2.14	0.44
1:A:97:ASN:ND2	1:A:99:SER:H	2.17	0.43
1:A:104:TYR:CD1	1:A:135:MET:CE	3.00	0.43
1:A:24:ALA:O	1:A:25:ASN:CB	2.66	0.43
1:A:70:GLY:HA3	1:A:208:THR:OG1	2.18	0.43
1:A:26:VAL:O	1:A:88:VAL:CG2	2.57	0.43
1:A:36:GLN:NE2	1:A:210:PRO:HA	2.34	0.42
1:A:163:ASN:ND2	4:A:856:HOH:O	2.51	0.42
1:A:47:GLY:HA3	1:A:92:ALA:O	2.19	0.42
1:A:62:ASN:HB2	1:A:98:SER:O	2.21	0.41
1:A:58:ASN:ND2	1:A:58:ASN:N	2.67	0.41
1:A:265:LYS:HG3	1:A:265:LYS:HZ2	1.30	0.41
1:A:234:ILE:HG21	1:A:234:ILE:HD13	1.77	0.41
1:A:265:LYS:HD2	1:A:265:LYS:HA	1.89	0.41
1:A:88:VAL:CG2	1:A:89:SER:N	2.83	0.41
1:A:62:ASN:ND2	1:A:64:HIS:HB2	2.35	0.41
1:A:67:HIS:CD2	1:A:217:LEU:HD22	2.55	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	A	273/274 (100%)	261 (96%)	12 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	199/198 (100%)	182 (92%)	17 (8%)	10	6

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	41	ASP
1	A	58	ASN
1	A	62	ASN
1	A	78	THR
1	A	97	ASN
1	A	98	SER
1	A	158	ASN
1	A	161	SER
1	A	163	ASN
1	A	190[A]	SER
1	A	190[B]	SER
1	A	217	LEU

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Mol	Chain	Res	Type
1	A	222	MET
1	A	240	ASN
1	A	249	ARG
1	A	265	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	36	GLN
1	A	58	ASN
1	A	62	ASN
1	A	97	ASN
1	A	141	ASN
1	A	158	ASN
1	A	163	ASN
1	A	212	ASN
1	A	238	HIS
1	A	240	ASN
1	A	245	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.