wwPDB X-ray Structure Validation Summary Report (i)

Feb 5, 2024 – 12:21 AM EST

PDB ID	:	1SCB
Title	:	ENZYME CRYSTAL STRUCTURE IN A NEAT ORGANIC SOLVENT
Authors	:	Fitzpatrick, P.A.; Steinmetz, A.C.U.; Ringe, D.; Klibanov, A.M.
Deposited on	:	1993-07-13
Resolution	:	2.30 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

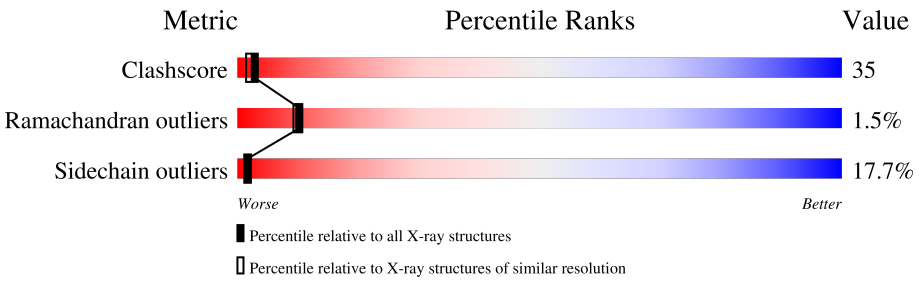
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	274	53% 35% 8% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CCN	A	404	-	-	X	-
3	CCN	A	406	-	-	X	-
3	CCN	A	408	-	-	X	-
3	CCN	A	409	-	-	X	-
3	CCN	A	413	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2056 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
			Total	C	N	O	S			
1	A	274	1920	1190	332	393	5	0	0	0

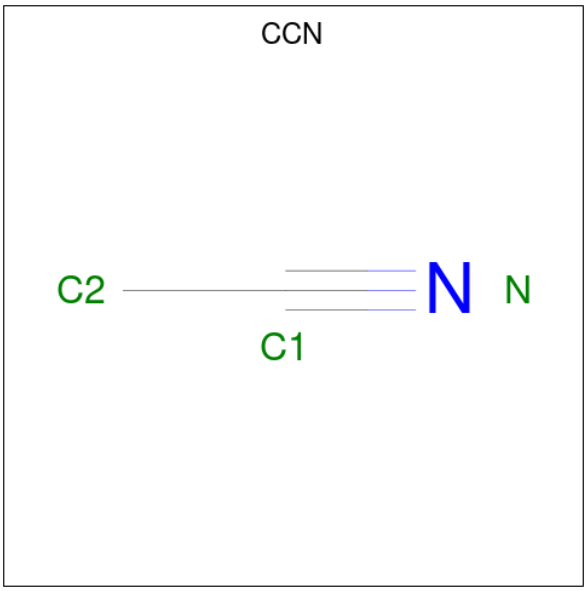
There are 5 discrepancies between the modelled and reference sequences:

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
			Total	Ca		
2	A	1	1	1	0	0

- Molecule 3 is ACETONITRILE (three-letter code: CCN) (formula: C_2H_3N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	3	2	1	0	0
			Total	C	N		
3	A	1	3	2	1	0	0
			Total	C	N		
3	A	1	3	2	1	0	0
			Total	C	N		
3	A	1	3	2	1	0	0
			Total	C	N		
3	A	1	3	2	1	0	0
			Total	C	N		
3	A	1	3	2	1	0	0
			Total	C	N		
3	A	1	3	2	1	0	0
			Total	C	N		
3	A	1	3	2	1	0	0
			Total	C	N		
3	A	1	3	2	1	0	0
			Total	C	N		
3	A	1	3	2	1	0	0
			Total	C	N		
3	A	1	3	2	1	0	0
			Total	C	N		
3	A	1	3	2	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	99	99	99	0	0

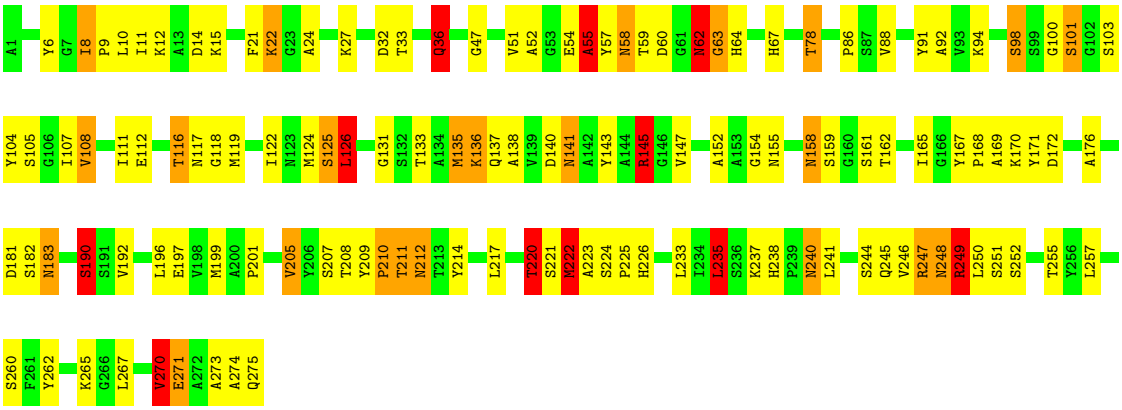
3 Residue-property plots (i)

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.

Note EDS was not executed.

• Molecule 1: SUBTILISIN CARLSBERG

Chain A: 53% 35% 8% •



4 Data and refinement statistics (i)

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	77.10Å 55.40Å 53.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2056	wwPDB-VP
Average B, all atoms (Å^2)	11.0	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: CCN, 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	1.07	6/1952 (0.3%)	1.70	30/2662 (1.1%)

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	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	ALA	C-N	17.28	1.73	1.34
1	A	112	GLU	CD-OE2	7.21	1.33	1.25
1	A	54	GLU	CD-OE1	6.95	1.33	1.25
1	A	190	SER	CB-OG	-6.29	1.34	1.42
1	A	271	GLU	CD-OE2	6.07	1.32	1.25

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	PRO	C-N-CA	17.28	164.91	121.70
1	A	249	ARG	NE-CZ-NH1	13.40	127.00	120.30
1	A	55	ALA	O-C-N	-13.18	101.61	122.70
1	A	125	SER	O-C-N	-12.48	102.73	122.70
1	A	126	LEU	N-CA-CB	9.14	128.67	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	SER	Mainchain,Peptide
1	A	249	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	A	1920	0	1879	135	0
2	A	1	0	0	0	0
3	A	36	0	36	14	0
4	A	99	0	0	8	0
All	All	2056	0	1915	136	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 35.

The worst 5 of 136 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:55:ALA:C	1:A:57:TYR:N	1.73	1.41
1:A:152:ALA:HB1	1:A:220:THR:HG23	1.33	1.08
1:A:8:ILE:HG13	1:A:9:PRO:HD3	1.35	1.07
1:A:111:ILE:HG23	4:A:362:HOH:O	1.56	1.02
1:A:27:LYS:HB2	1:A:27:LYS:HZ2	1.21	1.01

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	272/274 (99%)	258 (95%)	10 (4%)	4 (2%)	10 10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLY
1	A	126	LEU
1	A	55	ALA
1	A	36	GLN

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	198/198 (100%)	163 (82%)	35 (18%)	2 1

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	LEU
1	A	240	ASN
1	A	250	LEU
1	A	116	THR
1	A	108	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	185	ASN
1	A	248	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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	$\#\|Z\| > 2$
3	CCN	A	406	-	2,2,2	0.27	0	1,1,1	0.50	0
3	CCN	A	404	-	2,2,2	0.39	0	1,1,1	0.29	0
3	CCN	A	411	-	2,2,2	0.30	0	1,1,1	0.17	0
3	CCN	A	410	-	2,2,2	0.34	0	1,1,1	0.45	0
3	CCN	A	413	-	2,2,2	0.28	0	1,1,1	0.25	0
3	CCN	A	408	-	2,2,2	0.35	0	1,1,1	0.20	0
3	CCN	A	416	-	2,2,2	0.17	0	1,1,1	0.31	0
3	CCN	A	407	-	2,2,2	0.38	0	1,1,1	0.29	0
3	CCN	A	415	-	2,2,2	0.11	0	1,1,1	0.13	0
3	CCN	A	405	-	2,2,2	0.65	0	1,1,1	0.26	0
3	CCN	A	409	-	2,2,2	0.59	0	1,1,1	0.04	0
3	CCN	A	414	-	2,2,2	0.16	0	1,1,1	0.50	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.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	406	CCN	2	0
3	A	404	CCN	3	0
3	A	411	CCN	1	0
3	A	410	CCN	1	0
3	A	413	CCN	2	0
3	A	408	CCN	2	0
3	A	405	CCN	1	0
3	A	409	CCN	2	0

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	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	55:ALA	C	57:TYR	N	1.73

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.