



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:50 PM GMT

PDB ID : 1CQR
Title : CRYSTAL STRUCTURE OF THE STROMELYSIN CATALYTIC DOMAIN
AT 2.0 Å RESOLUTION
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Deposited on : 1999-08-11
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

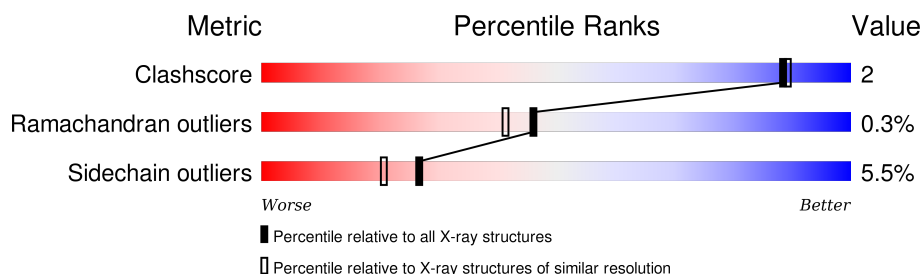
1 Overall quality at a glance

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	173	 84% 12% ...
1	B	173	 80% 16% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2814 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 STROMELYSIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1346	865	224	255	2			
1	B	173	Total	C	N	O	S	0	0	0
			1376	882	228	264	2			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	41	Total	O	0	0
			41	41		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: STROMELYSIN-1

Chain A: 



• Molecule 1: STROMELYSIN-1

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.20 Å 79.10 Å 107.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.00	Depositor
% Data completeness (in resolution range)	90.1 (12.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.199 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2814	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.90	0/1390	1.58	26/1899 (1.4%)
1	B	0.94	1/1421 (0.1%)	1.52	22/1941 (1.1%)
All	All	0.92	1/2811 (0.0%)	1.55	48/3840 (1.2%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	ASP	C-N	-7.05	1.17	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	TRP	CD1-CG-CD2	8.88	113.41	106.30
1	A	124	TRP	CD1-CG-CD2	8.87	113.39	106.30
1	A	186	TRP	CD1-CG-CD2	8.42	113.03	106.30
1	B	186	TRP	CD1-CG-CD2	8.38	113.00	106.30
1	A	92	TRP	CE2-CD2-CG	-8.19	100.75	107.30
1	A	168	TYR	CB-CG-CD2	-7.90	116.26	121.00
1	B	92	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	A	124	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	A	186	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	B	233	ARG	NE-CZ-NH1	7.26	123.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A	111	ASP	CA-CB-CG	7.14	129.12	113.40
1	B	186	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	B	107	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	124	TRP	CD1-CG-CD2	7.09	111.97	106.30
1	B	100	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	124	TRP	CE2-CD2-CG	-6.87	101.81	107.30
1	A	124	TRP	CG-CD2-CE3	6.75	139.98	133.90
1	B	232	PHE	CA-C-N	-6.40	103.13	117.20
1	A	181	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	230	THR	N-CA-C	-6.24	94.16	111.00
1	B	93	ARG	CA-CB-CG	6.21	127.06	113.40
1	A	107	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	111	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	92	TRP	CG-CD2-CE3	6.08	139.38	133.90
1	A	229	LEU	N-CA-C	5.99	127.16	111.00
1	A	124	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	B	186	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	B	153	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	93	ARG	CA-CB-CG	5.83	126.22	113.40
1	A	215	THR	N-CA-CB	-5.82	99.25	110.30
1	A	233	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	92	TRP	CG-CD2-CE3	5.75	139.07	133.90
1	A	124	TRP	CB-CG-CD1	-5.72	119.56	127.00
1	A	226	LEU	CA-CB-CG	5.67	128.33	115.30
1	A	233	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	92	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	B	155	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	A	92	TRP	CB-CG-CD1	-5.56	119.77	127.00
1	A	186	TRP	CG-CD1-NE1	-5.50	104.60	110.10
1	B	186	TRP	CG-CD2-CE3	5.47	138.82	133.90
1	B	177	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	125	GLU	CA-CB-CG	5.28	125.02	113.40
1	B	233	ARG	CA-CB-CG	5.26	124.98	113.40
1	A	162	ASN	CA-C-N	5.17	128.57	117.20
1	B	216	GLU	CA-CB-CG	5.17	124.77	113.40
1	B	94	LYS	CA-CB-CG	5.11	124.65	113.40
1	B	100	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	LEU	Peptide

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	1346	0	1270	4	0
1	B	1376	0	1294	10	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	41	0	0	0	0
4	B	41	0	0	0	0
All	All	2814	0	2564	13	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 2.

All (13) 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:B:214:ASN:OD1	1:B:216:GLU:HG3	1.97	0.65
1:B:115:SER:O	1:B:119:LYS:HG2	2.04	0.57
1:A:106:PRO:HD3	1:B:103:ASN:HA	1.97	0.47
1:A:228:ASP:O	1:A:230:THR:N	2.48	0.47
1:B:122:LYS:NZ	1:B:122:LYS:HB2	2.29	0.47
1:B:181:ASP:O	1:B:184:GLU:HG2	2.20	0.42
1:B:242:ILE:HD12	1:B:242:ILE:HA	1.88	0.42
1:A:194:ASN:HD21	1:A:196:PHE:HB3	1.85	0.42
1:B:228:ASP:O	1:B:229:LEU:C	2.54	0.42
1:B:214:ASN:O	1:B:220:TYR:HB2	2.19	0.41
1:A:230:THR:HG23	1:A:231:ARG:HH11	1.86	0.41
1:B:94:LYS:HD3	1:B:97:LEU:HD23	2.02	0.41
1:B:229:LEU:HB2	1:B:230:THR:OG1	2.21	0.40

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	167/173 (96%)	158 (95%)	8 (5%)	1 (1%)	30	22
1	B	171/173 (99%)	161 (94%)	10 (6%)	0	100	100
All	All	338/346 (98%)	319 (94%)	18 (5%)	1 (0%)	46	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	LEU

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	143/147 (97%)	138 (96%)	5 (4%)	43	40
1	B	147/147 (100%)	136 (92%)	11 (8%)	17	11
All	All	290/294 (99%)	274 (94%)	16 (6%)	27	21

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	THR
1	A	93	ARG
1	A	108	LEU
1	A	139	GLU
1	A	197	LEU

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Mol	Chain	Res	Type
1	B	95	THR
1	B	122	LYS
1	B	130	LEU
1	B	131	THR
1	B	215	THR
1	B	216	GLU
1	B	226	LEU
1	B	227	THR
1	B	230	THR
1	B	233	ARG
1	B	251	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	194	ASN
1	B	96	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.