Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 01:01 PM EDT

PDB ID	:	1N8O
Title	:	Crystal structure of a complex between bovine chymotrypsin and ecotin
Authors	:	Cambillau, C.; Spinelli, S.; Lauwereys, M.
Deposited on	:	2002-11-21
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

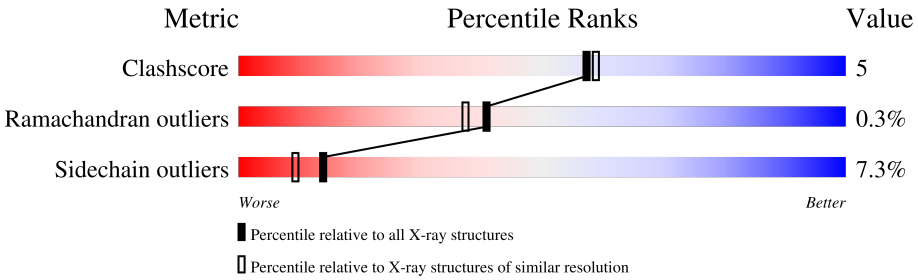
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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 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	A	13	77% 8% 15%
2	B	131	83% 12%
3	C	97	78% 18%
4	E	142	73% 18%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3009 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 Chymotrypsin A, A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	11	Total	C	N	O	S	0	0	0
			74	48	12	13	1			

- Molecule 2 is a protein called Chymotrypsin A, b chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			980	618	162	196	4			

- Molecule 3 is a protein called Chymotrypsin A, C chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	97	Total	C	N	O	S	0	0	0
			702	436	123	136	7			

- Molecule 4 is a protein called ecotin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	136	Total	C	N	O	S	0	0	0
			1036	664	173	193	6			

- Molecule 5 is water.

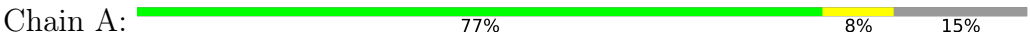
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	95	Total	O	0	0
			95	95		
5	C	45	Total	O	0	0
			45	45		
5	E	66	Total	O	0	0
			66	66		

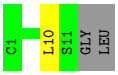
3 Residue-property plots (i)

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: Chymotrypsin A, A chain

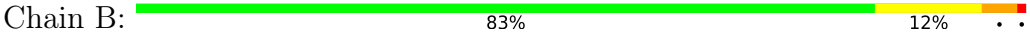
Chain A:

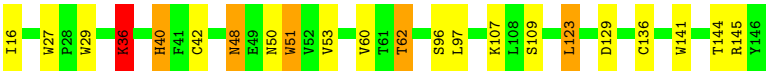




• Molecule 2: Chymotrypsin A, b chain

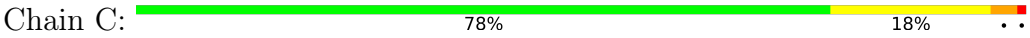
Chain B:

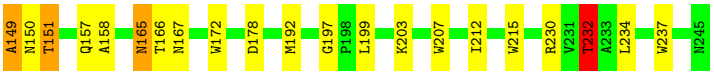




• Molecule 3: Chymotrypsin A, C chain

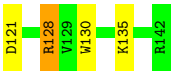
Chain C:





• Molecule 4: ecotin

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.50Å 63.80Å 79.60Å 90.00° 91.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 32.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 42.9 (32.08-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.205 , (Not available) 0.362 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.3	EDS
L-test for twinning[1]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	3009	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 100.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 0.0000e+00. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ 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	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.85	0/75	1.46	0/103
2	B	0.93	1/1000 (0.1%)	1.59	22/1361 (1.6%)
3	C	0.84	0/715	1.68	21/973 (2.2%)
4	E	0.82	0/1057	1.57	16/1438 (1.1%)
All	All	0.87	1/2847 (0.0%)	1.60	59/3875 (1.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	40	HIS	CB-CG	5.01	1.59	1.50

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	128	ARG	NE-CZ-NH2	9.95	125.28	120.30
2	B	27	TRP	CD1-CG-CD2	9.48	113.89	106.30
4	E	130	TRP	CD1-CG-CD2	8.87	113.40	106.30
2	B	141	TRP	CD1-CG-CD2	8.62	113.20	106.30
3	C	215	TRP	CD1-CG-CD2	8.42	113.04	106.30
3	C	151	THR	CA-CB-CG2	8.27	123.98	112.40
3	C	237	TRP	CD1-CG-CD2	8.23	112.89	106.30
4	E	67	TRP	CD1-CG-CD2	8.12	112.80	106.30
3	C	215	TRP	CE2-CD2-CG	-8.12	100.81	107.30
4	E	128	ARG	NE-CZ-NH1	-7.79	116.40	120.30
3	C	232	THR	N-CA-CB	-7.67	95.74	110.30
4	E	130	TRP	CE2-CD2-CG	-7.60	101.22	107.30
3	C	172	TRP	CD1-CG-CD2	7.60	112.38	106.30
2	B	36	LYS	CB-CG-CD	7.52	131.15	111.60
3	C	215	TRP	CG-CD2-CE3	7.47	140.63	133.90
2	B	62	THR	N-CA-CB	-7.38	96.28	110.30
4	E	54	ARG	CD-NE-CZ	7.37	133.91	123.60
2	B	27	TRP	CE2-CD2-CG	-7.27	101.48	107.30
4	E	108	ARG	NE-CZ-NH1	-7.22	116.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	207	TRP	CD1-CG-CD2	7.20	112.06	106.30
2	B	29	TRP	CD1-CG-CD2	7.14	112.01	106.30
2	B	141	TRP	CE2-CD2-CG	-7.11	101.61	107.30
2	B	51	TRP	CE2-CD2-CG	-7.00	101.70	107.30
3	C	237	TRP	CE2-CD2-CG	-6.97	101.73	107.30
4	E	54	ARG	NE-CZ-NH2	6.91	123.75	120.30
3	C	172	TRP	CE2-CD2-CG	-6.81	101.86	107.30
4	E	67	TRP	CE2-CD2-CG	-6.80	101.86	107.30
2	B	36	LYS	CA-CB-CG	-6.71	98.63	113.40
2	B	53	VAL	CG1-CB-CG2	-6.52	100.47	110.90
2	B	145	ARG	NE-CZ-NH1	-6.46	117.07	120.30
3	C	207	TRP	CE2-CD2-CG	-6.43	102.16	107.30
4	E	21	LYS	CB-CG-CD	-6.40	94.96	111.60
2	B	27	TRP	CG-CD1-NE1	-6.22	103.88	110.10
4	E	48	VAL	N-CA-CB	-5.98	98.34	111.50
4	E	77	VAL	CA-CB-CG2	-5.96	101.96	110.90
3	C	151	THR	CA-C-N	5.96	133.78	117.10
3	C	215	TRP	CB-CG-CD1	-5.96	119.26	127.00
3	C	234	LEU	CA-CB-CG	5.85	128.76	115.30
3	C	149	ALA	N-CA-C	-5.78	95.40	111.00
2	B	29	TRP	CE2-CD2-CG	-5.74	102.71	107.30
3	C	237	TRP	CG-CD1-NE1	-5.70	104.40	110.10
2	B	145	ARG	CD-NE-CZ	5.65	131.51	123.60
3	C	151	THR	CA-CB-OG1	-5.63	97.18	109.00
2	B	51	TRP	CD1-CG-CD2	5.46	110.67	106.30
2	B	51	TRP	CG-CD2-CE3	5.42	138.77	133.90
2	B	136	CYS	CA-CB-SG	-5.38	104.33	114.00
3	C	237	TRP	CG-CD2-CE3	5.34	138.71	133.90
4	E	13	TYR	CB-CG-CD2	-5.29	117.83	121.00
2	B	145	ARG	NE-CZ-NH2	5.29	122.94	120.30
3	C	151	THR	CA-C-O	-5.26	109.05	120.10
4	E	128	ARG	CB-CG-CD	-5.24	97.98	111.60
2	B	123	LEU	CA-CB-CG	5.24	127.35	115.30
2	B	141	TRP	CG-CD1-NE1	-5.24	104.86	110.10
3	C	199	LEU	N-CA-C	-5.18	97.02	111.00
4	E	113	LEU	CA-CB-CG	5.13	127.11	115.30
2	B	107	LYS	CA-CB-CG	-5.12	102.15	113.40
3	C	215	TRP	CG-CD1-NE1	-5.07	105.03	110.10
4	E	22	ARG	NE-CZ-NH2	5.05	122.82	120.30
2	B	141	TRP	CB-CG-CD1	-5.04	120.44	127.00

There are no chirality outliers.

There are no planarity outliers.

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	74	0	81	1	0
2	B	980	0	951	12	1
3	C	702	0	698	12	21
4	E	1036	0	1002	8	22
5	A	11	0	0	0	0
5	B	95	0	0	3	0
5	C	45	0	0	3	0
5	E	66	0	0	0	0
All	All	3009	0	2732	27	22

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 5.

All (27) 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)
2:B:48:ASN:HD22	2:B:50:ASN:H	1.28	0.82
2:B:36:LYS:HG2	5:B:232:HOH:O	2.00	0.61
2:B:36:LYS:O	2:B:36:LYS:HD3	2.04	0.58
2:B:40:HIS:H	3:C:149:ALA:HB2	1.72	0.55
4:E:59:LEU:HB2	4:E:101:LEU:HD22	1.90	0.54
2:B:48:ASN:HD21	2:B:51:TRP:HD1	1.58	0.52
3:C:232:THR:HB	5:C:250:HOH:O	2.10	0.52
5:B:148:HOH:O	3:C:197:GLY:HA3	2.12	0.50
2:B:48:ASN:HD22	2:B:50:ASN:N	2.04	0.47
2:B:48:ASN:ND2	2:B:50:ASN:H	2.02	0.47
3:C:165:ASN:ND2	3:C:230:ARG:HH11	2.12	0.47
3:C:149:ALA:N	3:C:150:ASN:OD1	2.47	0.47
2:B:16:ILE:HG21	3:C:158:ALA:HB2	1.97	0.45
3:C:178:ASP:HB3	5:C:285:HOH:O	2.17	0.45
1:A:10:LEU:HD13	3:C:157:GLN:NE2	2.31	0.45
2:B:60:VAL:HG23	5:B:157:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:57:GLY:HA3	4:E:74:PHE:CZ	2.52	0.44
3:C:150:ASN:OD1	4:E:86:ALA:HB1	2.19	0.43
4:E:25:ILE:HB	4:E:115:ILE:HB	2.00	0.43
3:C:232:THR:HG21	5:C:259:HOH:O	2.18	0.42
4:E:15:GLN:HA	4:E:22:ARG:HH11	1.84	0.42
2:B:16:ILE:O	2:B:144:THR:HA	2.20	0.42
2:B:40:HIS:HB3	3:C:149:ALA:HA	2.02	0.41
3:C:212:ILE:HD13	3:C:212:ILE:HG21	1.83	0.41
4:E:47:GLU:HA	4:E:93:GLU:O	2.21	0.41
2:B:42:CYS:SG	4:E:85:MET:HG2	2.60	0.41
4:E:22:ARG:HG3	4:E:118:TYR:CZ	2.56	0.41

All (22) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:THR:CG2	4:E:34:SER:OG[2_656]	0.57	1.63
3:C:166:THR:N	4:E:32:ASP:OD1[2_656]	0.65	1.55
3:C:166:THR:CA	4:E:32:ASP:OD1[2_656]	1.00	1.20
3:C:166:THR:CG2	4:E:34:SER:CB[2_656]	1.04	1.16
3:C:166:THR:CB	4:E:34:SER:OG[2_656]	1.15	1.05
3:C:166:THR:CA	4:E:32:ASP:CG[2_656]	1.39	0.81
3:C:165:ASN:CB	4:E:31:GLU:O[2_656]	1.52	0.68
3:C:166:THR:N	4:E:32:ASP:CG[2_656]	1.54	0.66
3:C:166:THR:OG1	4:E:34:SER:N[2_656]	1.64	0.56
3:C:166:THR:CA	4:E:32:ASP:OD2[2_656]	1.67	0.53
3:C:166:THR:CB	4:E:32:ASP:OD1[2_656]	1.84	0.36
2:B:129:ASP:OD2	4:E:112:LYS:NZ[2_656]	1.87	0.33
3:C:165:ASN:C	4:E:32:ASP:OD1[2_656]	1.87	0.33
3:C:166:THR:CB	4:E:34:SER:CB[2_656]	1.94	0.26
3:C:165:ASN:C	4:E:32:ASP:CG[2_656]	2.00	0.20
3:C:166:THR:CG2	4:E:34:SER:CA[2_656]	2.00	0.20
3:C:166:THR:CA	4:E:34:SER:OG[2_656]	2.04	0.16
3:C:178:ASP:OD2	4:E:31:GLU:N[2_656]	2.10	0.10
3:C:166:THR:OG1	4:E:32:ASP:C[2_656]	2.11	0.09
3:C:166:THR:OG1	4:E:32:ASP:OD1[2_656]	2.15	0.05
3:C:166:THR:OG1	4:E:32:ASP:O[2_656]	2.16	0.04
3:C:165:ASN:CG	4:E:31:GLU:O[2_656]	2.19	0.01

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	9/13 (69%)	9 (100%)	0	0	100 100
2	B	129/131 (98%)	124 (96%)	5 (4%)	0	100 100
3	C	95/97 (98%)	92 (97%)	2 (2%)	1 (1%)	14 8
4	E	132/142 (93%)	126 (96%)	6 (4%)	0	100 100
All	All	365/383 (95%)	351 (96%)	13 (4%)	1 (0%)	41 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	151	THR

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	9/10 (90%)	9 (100%)	0	100 100
2	B	109/109 (100%)	102 (94%)	7 (6%)	17 13
3	C	77/77 (100%)	72 (94%)	5 (6%)	17 12
4	E	107/125 (86%)	97 (91%)	10 (9%)	9 5
All	All	302/321 (94%)	280 (93%)	22 (7%)	14 9

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	36	LYS
2	B	48	ASN
2	B	62	THR
2	B	96	SER
2	B	97	LEU
2	B	109	SER
2	B	123	LEU
3	C	165	ASN
3	C	167	ASN
3	C	192	MET
3	C	203	LYS
3	C	232	THR
4	E	15	GLN
4	E	48	VAL
4	E	55	LEU
4	E	79	SER
4	E	98	THR
4	E	108	ARG
4	E	113	LEU
4	E	121	ASP
4	E	128	ARG
4	E	135	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	18	ASN
2	B	48	ASN
3	C	165	ASN
3	C	167	ASN
4	E	23	GLN
4	E	44	GLN
4	E	61	ASN
4	E	122	ASN

5.3.3 RNA

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)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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