wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2024 – 04:56 PM EDT

PDB ID	:	5CHA
Title	:	THE REFINEMENT AND THE STRUCTURE OF THE DIMER OF ALPHA-*CHYMOTRYPSIN AT 1.67-*ANGSTROMS RESOLUTION
Authors	:	Blevins, R.A.; Tulinsky, A.
Deposited on	:	1985-01-22
Resolution	:	1.67 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:

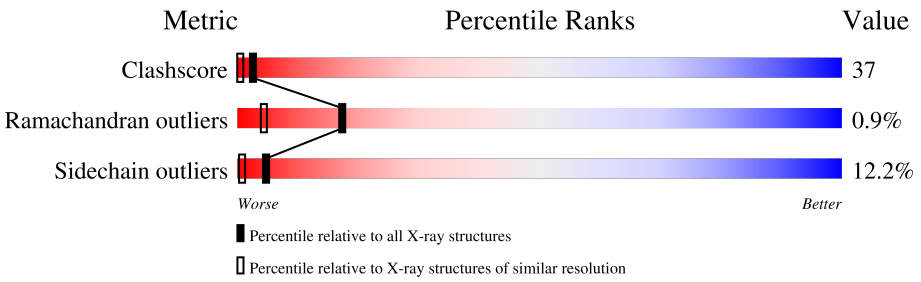
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.67 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	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)

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	13	23% 38% 8% 31%
1	E	13	46% 15% 8% 31%
2	B	131	41% 36% 18% 5%
2	F	131	47% 35% 14% 5%
3	C	97	51% 29% 16% •
3	G	97	52% 38% 7% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3719 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 ALPHA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	9	54	34	10	9	1	0	0	1
1	E	9	54	34	10	9	1	0	0	1

- Molecule 2 is a protein called ALPHA-CHYMOTRYPSIN A.

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

- Molecule 3 is a protein called ALPHA-CHYMOTRYPSIN A.

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	9	9	9	0	0
4	B	75	75	75	0	0
4	C	57	57	57	0	0
4	E	3	3	3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	F	59	59	59	0	0
			Total	O		
4	G	44	44	44	0	0

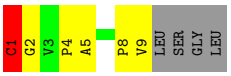
3 Residue-property plots (i)

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.

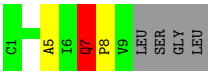
• Molecule 1: ALPHA-CHYMOTRYPSIN A

Chain A: 23% 38% 8% 31%



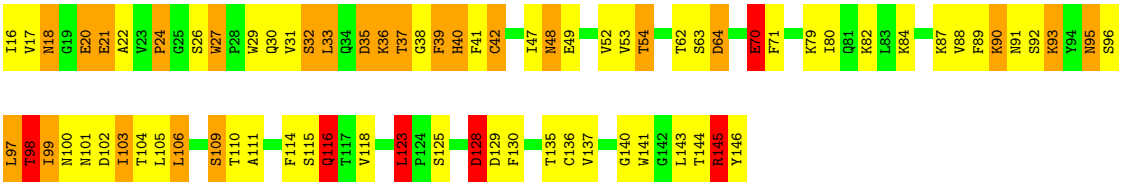
• Molecule 1: ALPHA-CHYMOTRYPSIN A

Chain E: 46% 15% 8% 31%



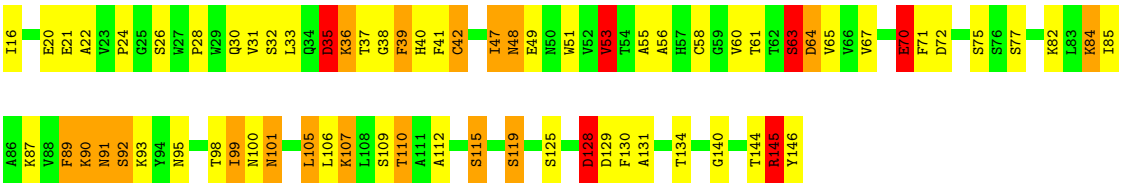
• Molecule 2: ALPHA-CHYMOTRYPSIN A

Chain B: 41% 36% 18% 5%



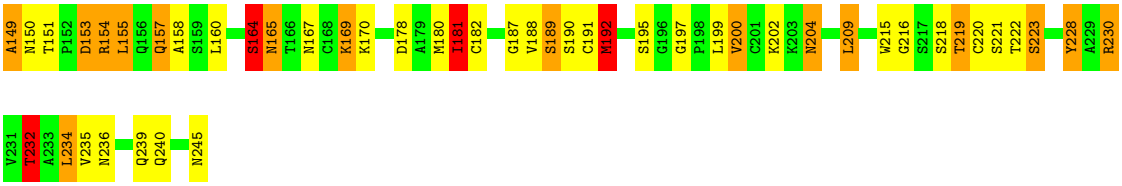
• Molecule 2: ALPHA-CHYMOTRYPSIN A

Chain F: 47% 35% 14% 5%



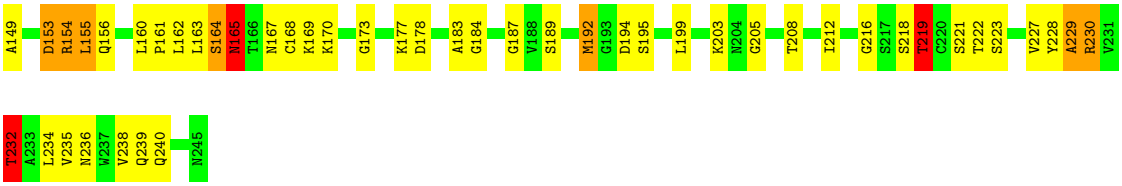
• Molecule 3: ALPHA-CHYMOTRYPSIN A

Chain C: 51% 29% 16% •



• Molecule 3: ALPHA-CHYMOTRYPSIN A

Chain G:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.29Å 67.48Å 65.94Å 90.00° 102.02° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.67	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.67)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3719	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

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	1.27	0/55	3.26	7/76 (9.2%)
1	E	1.06	0/55	2.11	2/76 (2.6%)
2	B	1.18	2/1000 (0.2%)	2.28	52/1361 (3.8%)
2	F	1.09	0/1000	2.22	38/1361 (2.8%)
3	C	1.37	2/715 (0.3%)	2.34	37/973 (3.8%)
3	G	1.27	1/715 (0.1%)	2.26	33/973 (3.4%)
All	All	1.21	5/3540 (0.1%)	2.29	169/4820 (3.5%)

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
2	F	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	154	ARG	NE-CZ	15.81	1.53	1.33
3	C	154	ARG	CG-CD	-6.29	1.36	1.51
3	G	223	SER	CB-OG	6.20	1.50	1.42
2	B	63	SER	CB-OG	5.89	1.50	1.42
2	B	146	TYR	CE1-CZ	5.25	1.45	1.38

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	178	ASP	CB-CG-OD1	17.25	133.82	118.30
3	C	230	ARG	NE-CZ-NH2	-15.04	112.78	120.30
2	F	128	ASP	CB-CG-OD1	14.81	131.63	118.30
3	C	228	TYR	CB-CG-CD2	-13.01	113.19	121.00
2	B	64	ASP	CB-CG-OD1	12.73	129.76	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	145	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	54	0	55	9	0
1	E	54	0	56	8	4
2	B	980	0	951	77	5
2	F	980	0	951	85	0
3	C	702	0	698	57	1
3	G	702	0	698	38	0
4	A	9	0	0	5	0
4	B	75	0	0	27	0
4	C	57	0	0	22	0
4	E	3	0	0	0	0
4	F	59	0	0	30	0
4	G	44	0	0	18	0
All	All	3719	0	3409	248	5

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 37.

The worst 5 of 248 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)
3:G:183:ALA:HB1	4:G:720:HOH:O	1.26	1.34
2:B:110:THR:HB	4:B:715:HOH:O	1.31	1.25
3:C:232:THR:HG23	4:C:681:HOH:O	1.40	1.19
3:C:235:VAL:HG22	4:C:627:HOH:O	1.44	1.16
3:C:221:SER:HB2	4:C:701:HOH:O	1.49	1.11

All (5) 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)
2:B:116:GLN:NE2	1:E:7:GLN:OE1[2_746]	1.47	0.73
2:B:116:GLN:CG	1:E:7:GLN:OE1[2_746]	1.55	0.65
2:B:116:GLN:CD	1:E:7:GLN:OE1[2_746]	1.90	0.30
2:B:116:GLN:NE2	1:E:7:GLN:CD[2_746]	2.11	0.09
2:B:79:LYS:CD	3:C:170:LYS:NZ[1_655]	2.17	0.03

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	7/13 (54%)	6 (86%)	0	1 (14%)	0 0
1	E	7/13 (54%)	7 (100%)	0	0	100 100
2	B	129/131 (98%)	124 (96%)	4 (3%)	1 (1%)	19 6
2	F	129/131 (98%)	123 (95%)	4 (3%)	2 (2%)	9 1
3	C	95/97 (98%)	92 (97%)	3 (3%)	0	100 100
3	G	95/97 (98%)	90 (95%)	5 (5%)	0	100 100
All	All	462/482 (96%)	442 (96%)	16 (4%)	4 (1%)	17 4

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLY
2	F	99	ILE
2	F	77	SER
2	B	99	ILE

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	6/10 (60%)	5 (83%)	1 (17%)	2 0
1	E	6/10 (60%)	5 (83%)	1 (17%)	2 0
2	B	109/109 (100%)	92 (84%)	17 (16%)	2 0
2	F	109/109 (100%)	93 (85%)	16 (15%)	3 0
3	C	77/77 (100%)	70 (91%)	7 (9%)	9 1
3	G	77/77 (100%)	72 (94%)	5 (6%)	17 4
All	All	384/392 (98%)	337 (88%)	47 (12%)	5 1

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	36	LYS
2	F	91	ASN
2	F	48	ASN
2	F	70	GLU
2	F	109	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	165	ASN
3	G	240	GLN
1	E	7	GLN
2	F	34	GLN
2	F	48	ASN

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)

There are no chain breaks in this entry.

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.