

Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 06:36 PM EST

PDB ID : 1CIQ

Title : COMPLEX OF TWO FRAGMENTS OF CI2, RESIDUES 1-40 AND 41-64

Authors : Buckle, A.M.; Fersht, A.R.

Deposited on : 1995-10-02

Resolution : 2.20 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 (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 (1)) 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)

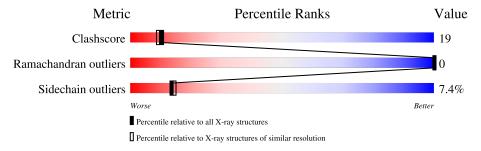
Validation Pipeline (wwPDB-VP) : 2.36

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 2.20 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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	40	52%	32%	8% 8%		
2	В	24	33%	54%	12%		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 535 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 INHIBITOR 2.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
1	A	37	Total 283	C 186	N 45	O 52	10	0	0

• Molecule 2 is a protein called CHYMOTRYPSIN INHIBITOR 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
2	В	24	Total 203	C 128	N 39	O 36	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	25	Total O 25 25	0	0
3	В	24	Total O 24 24	0	0

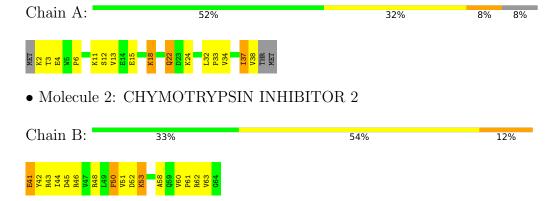


3 Residue-property plots (i)

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: CHYMOTRYPSIN INHIBITOR 2





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 6 2 2	Depositor	
Cell constants	69.17Å 69.17Å 53.91Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	7.00 - 2.20	Depositor	
% Data completeness	99.8 (7.00-2.20)	Depositor	
(in resolution range)	33.0 (1.00 2.20)		
R_{merge}	0.05	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	PROLSQ	Depositor	
R, R_{free}	0.180 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	535	wwPDB-VP	
Average B, all atoms (Å ²)	24.0	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	Bon	d lengths	Bond angles		
Moi Chain		RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	1.25	3/287 (1.0%)	2.20	10/390 (2.6%)	
2	В	1.15	2/205 (1.0%)	2.49	13/274 (4.7%)	
All	All	1.21	5/492 (1.0%)	2.32	23/664 (3.5%)	

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
1	A	37	ILE	CB-CG1	-10.44	1.24	1.54
1	A	11	LYS	CD-CE	-7.45	1.32	1.51
1	A	18	LYS	CD-CE	-7.44	1.32	1.51
2	В	41	GLU	CD-OE1	-6.37	1.18	1.25
2	В	41	GLU	CD-OE2	-6.02	1.19	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	45	ASP	CB-CG-OD1	14.16	131.05	118.30
1	A	18	LYS	CD-CE-NZ	11.19	137.44	111.70
2	В	45	ASP	CB-CG-OD2	-10.62	108.75	118.30
1	A	22	GLN	CB-CG-CD	10.03	137.68	111.60
2	В	62	ARG	NE-CZ-NH1	-9.79	115.41	120.30
2	В	52	ASP	CB-CG-OD2	8.09	125.58	118.30
1	A	38	VAL	CA-C-O	-7.64	104.06	120.10
1	A	4	GLU	OE1-CD-OE2	7.47	132.26	123.30
1	A	18	LYS	CB-CA-C	6.60	123.61	110.40
1	A	11	LYS	CG-CD-CE	6.45	131.24	111.90
2	В	41	GLU	OE1-CD-OE2	-6.41	115.61	123.30
1	A	37	ILE	O-C-N	6.09	132.45	122.70
2	В	41	GLU	N-CA-CB	-5.94	99.90	110.60
2	В	63	VAL	CA-CB-CG1	5.86	119.68	110.90
2	В	62	ARG	NE-CZ-NH2	5.73	123.17	120.30
2	В	61	PRO	C-N-CA	5.48	135.40	121.70
1	A	3	THR	O-C-N	5.14	130.92	122.70

Continued on next page...



Continued	trom	mromonie	maaa
-	110111	DICULUUS	pauc

Mol	Chain	Res	Type	Atoms	$f{Z} = f{Observed}(^o)$		$oxed{Ideal(^o)}$
1	A	24	LYS	CB-CA-C	5.13	120.66	110.40
2	В	42	TYR	CB-CG-CD2	5.12	124.07	121.00
1	A	2	LYS	CD-CE-NZ	5.04	123.30	111.70
2	В	50	PHE	C-N-CA	5.03	134.27	121.70
2	В	52	ASP	OD1-CG-OD2	-5.02	113.76	123.30
2	В	48	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	283	0	307	10	0
2	В	203	0	209	15	0
3	A	25	0	0	0	0
3	В	24	0	0	3	0
All	All	535	0	516	18	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 19.

All (18) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance } (\text{\AA}) \end{array}$	Clash overlap (Å)
1:A:12:SER:OG	1:A:15:GLU:HG3	1.75	0.87
2:B:44:ILE:O	2:B:44:ILE:HG13	1.92	0.69
1:A:6:PRO:HA	2:B:60:VAL:HG22	1.75	0.69
2:B:41:GLU:HG3	2:B:46:ARG:HH22	1.57	0.69
1:A:34:VAL:HG21	2:B:58:ALA:CB	2.24	0.68
1:A:34:VAL:CG2	2:B:58:ALA:HB3	2.27	0.64
2:B:43:ARG:CD	3:B:82:HOH:O	2.47	0.62
2:B:43:ARG:HD3	3:B:82:HOH:O	2.00	0.61
1:A:34:VAL:CG2	2:B:58:ALA:CB	2.79	0.60
2:B:43:ARG:HG3	2:B:46:ARG:NH2	2.18	0.59

Continued on next page...



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\operatorname{distance}\left(\operatorname{\mathring{A}} ight)$	$overlap (\AA)$
1:A:32:LEU:O	2:B:50:PHE:HA	2.05	0.56
2:B:43:ARG:HD2	3:B:82:HOH:O	2.09	0.51
1:A:12:SER:OG	1:A:15:GLU:CG	2.56	0.49
1:A:34:VAL:HG21	2:B:58:ALA:HB1	1.98	0.45
2:B:53:LYS:HE3	2:B:53:LYS:HB3	1.26	0.44
2:B:41:GLU:HG3	2:B:41:GLU:O	2.19	0.43
1:A:13:VAL:CG2	2:B:51:VAL:HG11	2.51	0.41
1:A:32:LEU:HA	1:A:33:PRO:HD3	1.79	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	Percenti	les
1	A	35/40 (88%)	34 (97%)	1 (3%)	0	100 10)0
2	В	22/24~(92%)	22 (100%)	0	0	100 10)0
All	All	57/64 (89%)	56 (98%)	1 (2%)	0	100 10)0

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	32/36 (89%)	29 (91%)	3 (9%)	8 8

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	В	22/22 (100%)	21 (96%)	1 (4%)	27 34
All	All	54/58 (93%)	50 (93%)	4 (7%)	13 14

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	22	GLN
1	A	37	ILE
2	В	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.

