



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3BG4 / pdb_00003bg4
Title : The crystal structure of guamerin in complex with chymotrypsin and the development of an elastase-specific inhibitor
Authors : Kim, H.; Chu, T.T.T.; Kim, D.Y.; Kim, D.R.; Nguyen, C.M.T.; Choi, J.; Lee, J.R.; Hahn, M.J.; Kim, K.K.
Deposited on : 2007-11-26
Resolution : 2.50 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

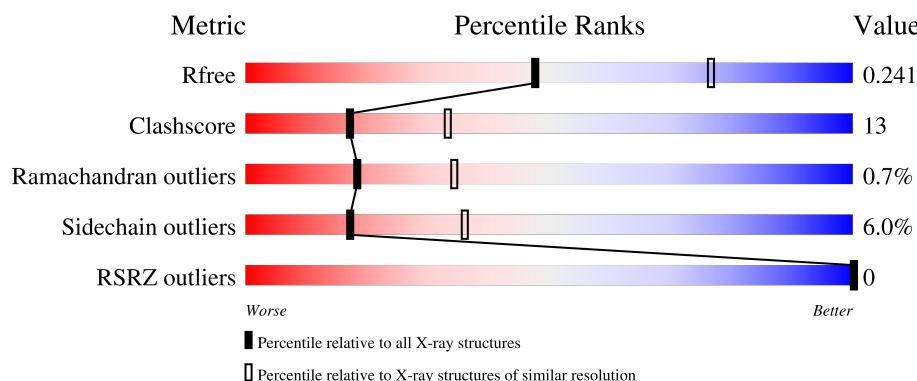
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	13	
2	B	131	
3	C	97	
4	D	57	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2172 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 chain A.

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 chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			979	618	162	195	4			

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

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 Guamerin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	46	Total	C	N	O	S	0	0	0
			335	201	56	67	11			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	36	Total	O	0	0
			36	36		
5	C	28	Total	O	0	0
			28	28		
5	D	14	Total	O	0	0
			14	14		

- Molecule 1: Chymotrypsin A chain A

[illegible]

A169	M160	T151	P152	D153	Q156	Q157	L160	P161	L162	M167	K170	K171	M170	M172	K175	G187	M192	S196	G196	G197	P198	C201	C202	K203	K204	G205	A206	V210	V213	G214	V215	T219	T222	V227	V228	A229	R230	V231	T232	A233	L234	V238	Q239	V245
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	VAL
ASP	
GLU	
ASN	
ALA	
GLU	
ASP	
THR	
HIS	
GLY	
LEU	
C12	
G13	
E14	
K15	
L24	
N25	
I33	
M36	
F43	
K44	
V45	
N48	
E51	
C54	
T55	
C56	
A57	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.27 Å 43.99 Å 122.57 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.50 29.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	80.0 (29.94-2.50) 80.0 (29.94-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.45 (at 2.51 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.187 , 0.241 0.187 , 0.241	Depositor DCC
R_{free} test set	399 reflections (5.43%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.054 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2172	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.46	0/75	1.13	0/103
2	B	0.38	0/999	0.96	5/1361 (0.4%)
3	C	0.46	0/715	1.01	3/973 (0.3%)
4	D	0.44	0/340	0.90	1/458 (0.2%)
All	All	0.42	0/2129	0.98	9/2895 (0.3%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	27	TRP	CA-C-N	10.15	130.44	119.28
2	B	27	TRP	C-N-CA	10.15	130.44	119.28
3	C	196	GLY	N-CA-C	-7.67	105.95	115.08
3	C	206	ALA	N-CA-C	7.01	120.88	109.59
2	B	109	SER	N-CA-C	-6.35	103.62	112.45
4	D	54	CYS	N-CA-C	5.50	119.14	111.56
2	B	49	GLU	N-CA-C	5.47	118.00	111.71
3	C	204	ASN	N-CA-CB	5.43	119.66	110.49
2	B	51	TRP	N-CA-C	5.07	117.51	109.50

There are no chirality outliers.

There are no planarity outliers.

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	74	0	81	4	0
2	B	979	0	951	30	0
3	C	702	0	698	26	0
4	D	335	0	301	4	0
5	A	4	0	0	0	0
5	B	36	0	0	3	0
5	C	28	0	0	1	0
5	D	14	0	0	0	0
All	All	2172	0	2031	52	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 13.

All (52) 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:65:VAL:HG11	2:B:82:LYS:HG3	1.59	0.84
1:A:10:LEU:HD23	3:C:157:GLN:NE2	1.96	0.79
4:D:43:PHE:HB2	4:D:51:GLU:HG2	1.69	0.74
3:C:232:THR:HG23	5:C:12:HOH:O	1.95	0.66
2:B:56:ALA:HA	2:B:104:THR:OG1	1.98	0.64
2:B:70:GLU:OE1	2:B:73:GLN:HA	2.00	0.62
2:B:105:LEU:HD21	3:C:238:VAL:HG13	1.82	0.62
2:B:28:PRO:HB2	2:B:119:SER:HB2	1.82	0.62
3:C:195:SER:HA	3:C:213:VAL:HB	1.86	0.58
2:B:129:ASP:HB2	5:B:173:HOH:O	2.05	0.56
3:C:160:LEU:HD12	3:C:160:LEU:N	2.22	0.55
2:B:144:THR:C	2:B:145:ARG:HG2	2.32	0.54
2:B:65:VAL:HG11	2:B:82:LYS:CG	2.36	0.53
1:A:8:PRO:HG3	2:B:26:SER:O	2.11	0.51
2:B:141:TRP:O	3:C:151:THR:HG23	2.11	0.50
2:B:33:LEU:HD22	2:B:66:VAL:HG22	1.95	0.49
2:B:74:GLY:HA3	3:C:153:ASP:OD2	2.13	0.49
4:D:14:GLU:O	4:D:15:LYS:HB3	2.13	0.48
2:B:65:VAL:HG21	2:B:82:LYS:HE3	1.96	0.48
2:B:45:SER:OG	3:C:198:PRO:HB3	2.14	0.48
5:B:163:HOH:O	3:C:156:GLN:HB2	2.14	0.48
1:A:5:ALA:HB2	5:B:172:HOH:O	2.13	0.48
3:C:172:TRP:O	3:C:175:LYS:NZ	2.46	0.47
4:D:24:LEU:O	4:D:25:ASN:HB3	2.14	0.47
2:B:56:ALA:O	2:B:90:LYS:HE2	2.15	0.47
2:B:29:TRP:CG	2:B:121:VAL:HB	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:ARG:O	3:C:234:LEU:HD22	2.15	0.47
2:B:146:TYR:CD2	3:C:219:THR:HA	2.51	0.46
3:C:201:CYS:SG	3:C:210:VAL:HG21	2.55	0.46
2:B:99:ILE:HG22	2:B:99:ILE:O	2.17	0.45
1:A:2:GLY:O	1:A:4:PRO:HD3	2.16	0.45
2:B:29:TRP:CD2	2:B:121:VAL:HB	2.52	0.45
3:C:215:TRP:CZ3	4:D:33:ILE:HD12	2.53	0.44
2:B:18:ASN:ND2	3:C:222:THR:HG21	2.33	0.44
2:B:95:ASN:ND2	2:B:98:THR:HG23	2.33	0.44
3:C:228:TYR:CD1	3:C:228:TYR:N	2.86	0.44
3:C:195:SER:C	3:C:197:GLY:H	2.26	0.44
2:B:67:VAL:HG13	2:B:80:ILE:HD12	1.99	0.43
3:C:203:LYS:O	3:C:204:ASN:C	2.61	0.43
2:B:17:VAL:O	2:B:18:ASN:HB2	2.17	0.43
2:B:146:TYR:CE2	3:C:219:THR:HA	2.53	0.43
3:C:167:ASN:C	3:C:167:ASN:HD22	2.26	0.43
3:C:215:TRP:CH2	3:C:227:VAL:HG21	2.54	0.42
2:B:91:ASN:HB2	2:B:103:ILE:HG23	2.02	0.42
2:B:24:PRO:HG3	2:B:71:PHE:CE2	2.55	0.42
2:B:18:ASN:HD22	3:C:222:THR:HG21	1.85	0.42
3:C:187:GLY:HA2	3:C:222:THR:HB	2.02	0.41
2:B:116:GLN:HE21	2:B:116:GLN:HB3	1.56	0.41
3:C:215:TRP:CZ2	3:C:227:VAL:HG21	2.55	0.41
2:B:134:THR:HB	3:C:162:LEU:HD12	2.03	0.41
3:C:170:LYS:HD3	3:C:171:TYR:CZ	2.56	0.41
2:B:31:VAL:HG22	2:B:44:GLY:C	2.46	0.41

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	9/13 (69%)	9 (100%)	0	0	100	100
2	B	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
3	C	95/97 (98%)	92 (97%)	2 (2%)	1 (1%)	11	22
4	D	44/57 (77%)	40 (91%)	3 (7%)	1 (2%)	5	8
All	All	277/298 (93%)	264 (95%)	11 (4%)	2 (1%)	18	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	204	ASN
4	D	36	MET

5.3.2 Protein sidechains ⓘ

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%)	104 (95%)	5 (5%)	24	48
3	C	77/77 (100%)	72 (94%)	5 (6%)	15	32
4	D	39/48 (81%)	35 (90%)	4 (10%)	7	14
All	All	234/244 (96%)	220 (94%)	14 (6%)	17	36

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	36	LYS
2	B	79	LYS
2	B	105	LEU
2	B	145	ARG
2	B	146	TYR
3	C	151	THR
3	C	160	LEU
3	C	192	MET
3	C	234	LEU

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Mol	Chain	Res	Type
3	C	239	GLN
4	D	14	GLU
4	D	45	VAL
4	D	48	ASN
4	D	55	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	34	GLN
2	B	73	GLN
2	B	95	ASN
2	B	116	GLN
3	C	150	ASN
3	C	165	ASN
3	C	167	ASN
3	C	240	GLN
3	C	245	ASN
4	D	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 oligosaccharides 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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	11/13 (84%)	0.12	0 100 100	23, 28, 39, 41	0
2	B	131/131 (100%)	-0.25	0 100 100	14, 24, 41, 50	0
3	C	97/97 (100%)	-0.27	0 100 100	13, 24, 39, 47	0
4	D	46/57 (80%)	-0.06	0 100 100	17, 27, 48, 55	0
All	All	285/298 (95%)	-0.22	0 100 100	13, 25, 41, 55	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.