Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 07:09 AM EDT

PDB ID	:	3BG4
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 (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:

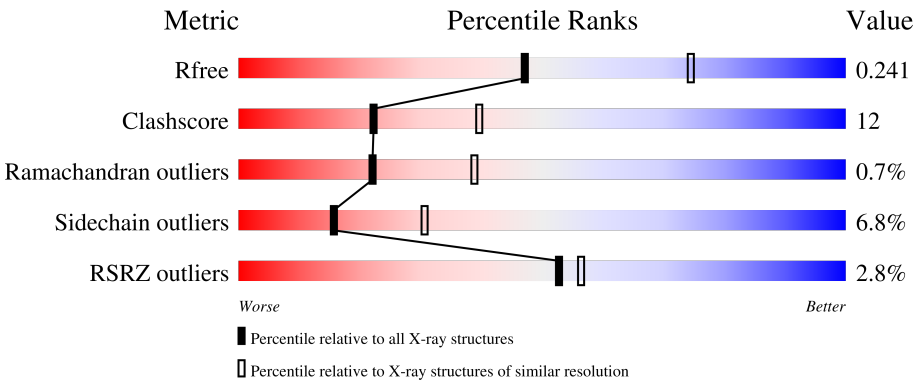
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	46% 38% 15%
2	B	131	2% 72% 26% •
3	C	97	3% 68% 28% •
4	D	57	4% 63% 16% • 19%

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
			Total	C	N	O	S			
1	A	11	74	48	12	13	1	0	0	0

- Molecule 2 is a protein called Chymotrypsin A chain B.

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

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

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

- Molecule 4 is a protein called Guamerin.

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

- Molecule 5 is water.

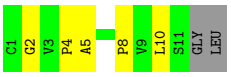
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	4	4	4	0	0
5	B	36	36	36	0	0
5	C	28	28	28	0	0
5	D	14	14	14	0	0

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 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.

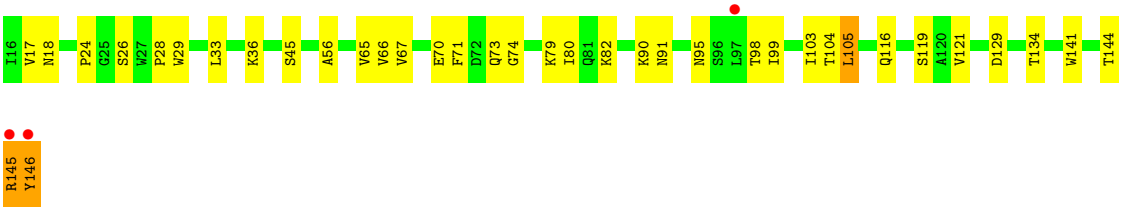
• Molecule 1: Chymotrypsin A chain A

Chain A: 46% 38% 15%



• Molecule 2: Chymotrypsin A chain B

Chain B: 2% 72% 26%

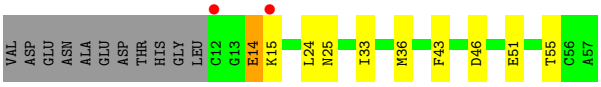


• Molecule 3: Chymotrypsin A chain C

Chain C: 3% 68% 28%

• Molecule 4: Guamerin

Chain D: 4% 63% 16% 19%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.27Å 43.99Å 122.57Å 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) 80.1 (29.94-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	5.45 (at 2.51Å)	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)	0.37 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]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	0.29	0/75	0.62	0/103
2	B	0.33	0/999	0.61	0/1361
3	C	0.34	0/715	0.71	1/973 (0.1%)
4	D	0.36	0/340	0.65	0/458
All	All	0.34	0/2129	0.65	1/2895 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	204	ASN	N-CA-CB	5.04	119.66	110.60

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	4	0
2	B	979	0	951	29	0
3	C	702	0	698	23	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2172	0	2031	48	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 12.

All (48) 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: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:144:THR:C	2:B:145:ARG:HG2	2.32	0.49
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:67:VAL:HG13	2:B:80:ILE:HD12	1.99	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: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

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%)	14	26
4	D	44/57 (77%)	40 (91%)	3 (7%)	1 (2%)	6	10
All	All	277/298 (93%)	264 (95%)	11 (4%)	2 (1%)	22	39

All (2) Ramachandran outliers are listed below:

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

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%)	104 (95%)	5 (5%)	27	50
3	C	77/77 (100%)	69 (90%)	8 (10%)	7	13
4	D	39/48 (81%)	36 (92%)	3 (8%)	13	25
All	All	234/244 (96%)	218 (93%)	16 (7%)	16	30

All (16) 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	165	ASN
3	C	167	ASN
3	C	191	CYS
3	C	192	MET
3	C	234	LEU
3	C	239	GLN
4	D	14	GLU
4	D	46	ASP
4	D	55	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	18	ASN
2	B	73	GLN
2	B	95	ASN
2	B	116	GLN
3	C	165	ASN
3	C	167	ASN
3	C	239	GLN
3	C	240	GLN
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 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)

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%)	0.07	0	100	100	23, 28, 39, 41	0
2	B	131/131 (100%)	-0.26	3 (2%)	60	63	14, 24, 41, 50	0
3	C	97/97 (100%)	-0.22	3 (3%)	49	52	13, 24, 39, 47	0
4	D	46/57 (80%)	-0.14	2 (4%)	35	38	17, 27, 48, 55	0
All	All	285/298 (95%)	-0.21	8 (2%)	53	56	13, 25, 41, 55	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	15	LYS	3.3
2	B	146	TYR	3.2
3	C	150	ASN	3.0
3	C	204	ASN	2.7
3	C	149	ALA	2.6
4	D	12	CYS	2.4
2	B	145	ARG	2.3
2	B	97	LEU	2.2

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 monosaccharides 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.