

wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 07:59 am BST

PDB ID : 6HGD

Title: Crystal structure of Alpha1-antichymotrypsin variant NewBG-0: a new

binding globulin variant that is devoid of any cortisol-binding capabilities

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Deposited on : 2018-08-23

Resolution : 1.90 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 following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \ (Phenix) & : & 1.13 \end{array}$

EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

 $\begin{array}{cccc} & CCP4 & : & 7.0.044 \; (Gargrove) \\ Ideal \; geometry \; (proteins) & : & Engh \; \& \; Huber \; (2001) \end{array}$

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

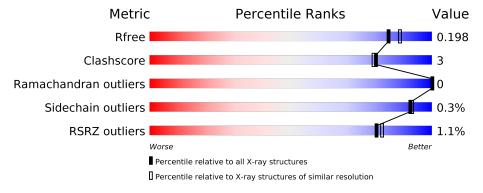
Validation Pipeline (wwPDB-VP) : 2.11

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 1.90 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	$\begin{array}{c} \textbf{Whole archive} \\ (\# \textbf{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	369	85%	6%	9%
2	В	40	90%		8%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3378 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-1-antichymotrypsin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	336	Total	С	N	О	S	0	4	0
	A	330	2676	1714	435	516	11	0	4	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP P01011
A	-7	LYS	-	expression tag	UNP P01011
A	-6	HIS	_	expression tag	UNP P01011
A	-5	HIS	-	expression tag	UNP P01011
A	-4	HIS	_	expression tag	UNP P01011
A	-3	HIS	_	expression tag	UNP P01011
A	-2	HIS	_	expression tag	UNP P01011
A	-1	HIS	_	expression tag	UNP P01011
A	0	MET	_	expression tag	UNP P01011
A	1	LYS	_	expression tag	UNP P01011
A	2	GLN	_	expression tag	UNP P01011
A	24	ARG	LEU	engineered mutation	UNP P01011
A	242	GLN	GLU	engineered mutation	UNP P01011
A	244	ASN	LYS	engineered mutation	UNP P01011
A	274	ASN	LYS	engineered mutation	UNP P01011
A	277	GLY	ARG	engineered mutation	UNP P01011

• Molecule 2 is a protein called Alpha-1-antichymotrypsin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	B	27	Total	С	N	О	S	0	0	0
	Б	31	317	210	55	50	2	0	U	U

There are 4 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
В	382	ASP	PRO	engineered mutation	UNP P01011
В	383	HIS	THR	engineered mutation	UNP P01011
В	384	PHE	ASP	engineered mutation	UNP P01011
В	386	TRP	GLN	engineered mutation	UNP P01011

• Molecule 3 is water.

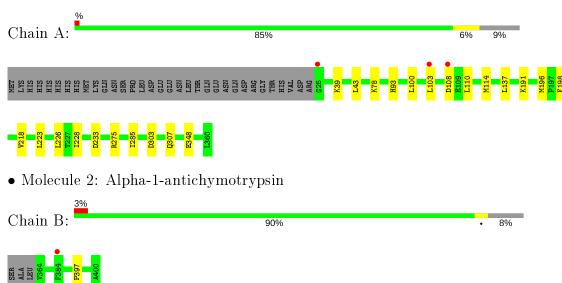
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	348	Total O 348 348	0	0
3	В	37	Total O 37 37	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Alpha-1-antichymotrypsin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	41.55Å 93.13Å 49.33Å	Depositor
a, b, c, α , β , γ	90.00° 110.42° 90.00°	Depositor
Resolution (Å)	38.94 - 1.90	Depositor
resolution (11)	41.41 - 1.90	EDS
% Data completeness	99.4 (38.94-1.90)	Depositor
(in resolution range)	99.4 (41.41-1.90)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	5.06 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
P. P.	0.147 , 0.198	Depositor
R, R_{free}	0.147 , 0.198	DCC
R_{free} test set	1379 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 54.9	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3378	wwPDB-VP
Average B, all atoms $(Å^2)$	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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		
WIOI	Chain	RMSZ # Z		RMSZ	# Z >5	
1	Α	0.38	0/2738	0.55	0/3702	
2	В	0.40	0/326	0.51	0/441	
All	All	0.38	0/3064	0.55	0/4143	

There are no bond length outliers.

There are no bond angle outliers.

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	2676	0	2686	16	0
2	В	317	0	323	1	0
3	A	348	0	0	2	0
3	В	37	0	0	0	0
All	All	3378	0	3009	16	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 3.

The worst 5 of 16 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{l} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:A:78:LYS:NZ	3:A:406:HOH:O	2.36	0.59

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Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:A:103:LEU:HD12	1:A:114:MET:CE	2.33	0.59
1:A:103:LEU:HD12	1:A:114:MET:HE2	1.88	0.56
1:A:100:LEU:HD23	1:A:114:MET:HE3	1.89	0.55
1:A:110:LEU:HD23	1:A:110:LEU:C	2.28	0.55

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	Perce	\mathbf{ntiles}
1	A	338/369 (92%)	333 (98%)	5 (2%)	0	100	100
2	В	35/40 (88%)	35 (100%)	0	0	100	100
All	All	373/409 (91%)	368 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	298/326 (91%)	297 (100%)	1 (0%)	92 93
2	В	$36/38 \; (95\%)$	36 (100%)	0	100 100
All	All	334/364 (92%)	333 (100%)	1 (0%)	92 93



All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASP

Some 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 carbohydrates 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, 95^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	336/369 (91%)	-0.67	3 (0%) 84 85	8, 17, 34, 58	0
2	В	37/40 (92%)	-0.40	1 (2%) 54 57	10, 16, 42, 49	0
All	All	373/409 (91%)	-0.65	4 (1%) 80 82	8, 17, 37, 58	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	GLY	3.9
2	В	384	PHE	3.5
1	A	103	LEU	3.0
1	A	108	ASP	2.3

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 carbohydrates 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.

