

Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 10:11 AM EDT

PDB ID : 6C6G

Title : An unexpected vestigial protein complex reveals the evolutionary origins of an

s-triazine catabolic enzyme. Inhibitor bound complex.

Authors: Peat, T.S.; Esquirol, L.; Wilding, M.; Liu, J.W.; French, N.G.; Hartley, C.J.;

Hideki, O.; Easton, C.J.; Newman, J.; Scott, C.

Deposited on : 2018-01-18

Resolution : 2.10 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

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35.1

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

 $Refmac \quad : \quad 5.8.0158$

 $\begin{tabular}{lll} CCP4 & : & 7.0.044 & (Gargrove) \end{tabular}$

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

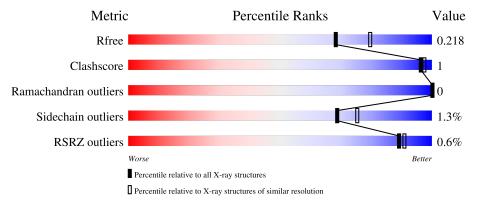
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 2.10 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	$(\# ext{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$		
R_{free}	130704	5197 (2.10-2.10)		
Clashscore	141614	5710 (2.10-2.10)		
Ramachandran outliers	138981	5647 (2.10-2.10)		
Sidechain outliers	138945	5648 (2.10-2.10)		
RSRZ outliers	127900	5083 (2.10-2.10)		

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	457	96%		•
1	В	457	95%		•
2	С	68	87%	10%	
2	D	68	90%	7%	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8523 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 Biuret hydrolase.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	A	457	Total 3439	C 2164	N 622	O 637	P 1	S 15	0	7	0
1	В	457	Total 3434	C 2160	N 625	O 633	P 1	S 15	0	5	0

• Molecule 2 is a protein called AtzG.

\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
2	С	66	Total	С	N	О	S	0	0	0	
		00	503	324	82	96	1	U			
2	D	D	66	Total	С	N	О	S	0	0	0
	00	506	326	82	96	2		0	U		

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	В	1	Total Ca 1 1	0	0

• Molecule 4 is water.

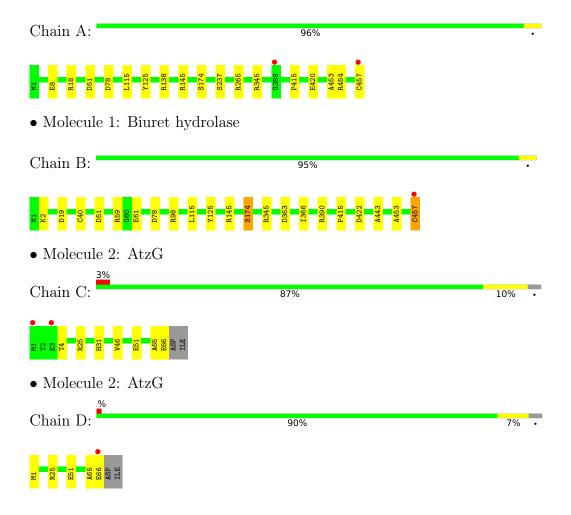
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	261	Total O 261 261	0	0
4	В	284	Total O 284 284	0	0
4	С	39	Total O 39 39	0	0
4	D	55	Total O 55 55	0	0



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: Biuret hydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants	78.63Å 88.91Å 141.85Å	Donositor
a, b, c, α , β , γ	90.00° 101.32° 90.00°	Depositor
Resolution (Å)	74.91 - 2.10	Depositor
Resolution (A)	69.55 - 2.10	EDS
% Data completeness	100.0 (74.91-2.10)	Depositor
(in resolution range)	100.0 (69.55-2.10)	EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.02 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
D D.	0.166 , 0.210	Depositor
R, R_{free}	0.179 , 0.218	DCC
R_{free} test set	2726 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 48.9	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8523	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.44% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SVV

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	Boı	nd lengths	В	ond angles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	A	0.72	1/3502~(0.0%)	0.84	10/4777 (0.2%)
1	В	0.73	0/3497	0.88	7/4767 (0.1%)
2	С	0.77	0/516	0.88	1/706 (0.1%)
2	D	0.83	0/519	0.84	1/709 (0.1%)
All	All	0.74	1/8034 (0.0%)	0.86	19/10959 (0.2%)

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
1	A	0	1
1	В	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	A	237	SER	CB-OG	-5.26	1.35	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
1	A	345	ARG	NE-CZ-NH1	7.59	124.10	120.30
2	С	25	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	В	363	ASP	CB-CG-OD1	6.64	124.28	118.30
2	D	25	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	В	457	CYS	CA-CB-SG	6.35	125.43	114.00
1	A	51	ASP	CB-CG-OD1	6.33	123.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
1	В	390	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	В	51	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	265	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	В	78	ASP	CB-CG-OD1	5.84	123.55	118.30
1	В	19	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	138	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	345	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	145	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	78	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	В	145	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	18	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	A	18	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	A	454	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	420	GLU	Peptide
1	В	174	SVV	Mainchain

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	3439	0	3447	3	0
1	В	3434	0	3450	7	0
2	С	503	0	497	5	0
2	D	506	0	504	2	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
4	A	261	0	0	0	1
4	В	284	0	0	0	1
4	С	39	0	0	1	0
4	D	55	0	0	1	0
All	All	8523	0	7898	15	1



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 1.

All (15) 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:C:51:GLU:OE1	4:C:101:HOH:O	2.08	0.71
2:D:51:GLU:OE1	4:D:101:HOH:O	2.10	0.68
1:B:98[B]:ARG:CG	1:B:98[B]:ARG:O	2.45	0.65
1:B:345:ARG:NH2	2:C:46:VAL:O	2.38	0.55
1:B:59[B]:ARG:NH2	1:B:61:GLU:OE1	2.42	0.52
1:B:98[B]:ARG:O	1:B:98[B]:ARG:HG2	2.11	0.50
2:D:65:ALA:O	2:D:66:GLU:HB2	2.12	0.49
1:B:366[B]:ILE:HD13	1:B:443:ALA:HB2	1.95	0.49
2:C:65:ALA:O	2:C:66:GLU:HB2	2.15	0.47
1:A:415:PRO:O	1:A:453:ALA:HA	2.15	0.47
1:B:98[B]:ARG:O	1:B:98[B]:ARG:HG3	2.14	0.46
1:A:8:GLU:CD	2:C:31:HIS:HD1	2.14	0.46
1:B:415:PRO:O	1:B:453:ALA:HA	2.15	0.45
2:C:66:GLU:HA	2:C:66:GLU:OE1	2.16	0.45
1:A:115[A]:LEU:HD23	1:A:115[A]:LEU:HA	1.84	0.43

All (1) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
4:A:697:HOH:O	4:B:871:HOH:O[3_544]	2.06	0.14

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	461/457 (101%)	450 (98%)	11 (2%)	0	100 100	

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	$459/457 \; (100\%)$	446 (97%)	13 (3%)	0	100	100
2	С	64/68 (94%)	62 (97%)	2 (3%)	0	100	100
2	D	64/68 (94%)	63 (98%)	1 (2%)	0	100	100
All	All	1048/1050 (100%)	1021 (97%)	27 (3%)	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	351/345 (102%)	349 (99%)	2 (1%)	86 90
1	В	350/345~(101%)	343 (98%)	7 (2%)	55 60
2	С	51/54 (94%)	50 (98%)	1 (2%)	55 60
2	D	52/54 (96%)	51 (98%)	1 (2%)	57 63
All	All	804/798 (101%)	793 (99%)	11 (1%)	69 73

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	TYR
1	A	457	CYS
1	В	2	LYS
1	В	40	CYS
1	В	115[A]	LEU
1	В	115[B]	LEU
1	В	125	TYR
1	В	422	ASP
1	В	457	CYS
2	С	4	THR
2	D	1	MET

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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type Cl		Chain	Dog	Dog	Dog	Dec	Dag	Dag	Pos	Res	Pos	Des	Dan	Das	Timle	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2											
1	SVV	A	174	1	7,9,10	2.05	3 (42%)	5,12,14	1.95	2 (40%)											
1	SVV	В	174	1	7,9,10	2.10	3 (42%)	5,12,14	3.29	2 (40%)											

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SVV	A	174	1	-	1/3/8/10	-
1	SVV	В	174	1	-	2/3/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(ext{\AA})$
1	В	174	SVV	P1-O2	3.23	1.51	1.46
1	В	174	SVV	P1-O3	-3.16	1.48	1.56
1	A	174	SVV	P1-O3	-2.99	1.48	1.56
1	A	174	SVV	O-C	2.50	1.29	1.19
1	A	174	SVV	P1-O2	2.14	1.49	1.46
1	В	174	SVV	O-C	2.07	1.28	1.19

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	174	SVV	OG-CB-CA	-6.68	101.64	108.14
1	A	174	SVV	OG-P1-O2	-3.43	104.36	115.61
1	В	174	SVV	OG-P1-O2	-2.90	106.09	115.61
1	A	174	SVV	OG-CB-CA	-2.05	106.15	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	174	SVV	CB-OG-P1-O2
1	В	174	SVV	N-CA-CB-OG
1	В	174	SVV	CB-OG-P1-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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></rsrz>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	456/457~(99%)	-0.48	2 (0%) 92 93	9, 15, 29, 56	1 (0%)
1	В	456/457 (99%)	-0.56	1 (0%) 95 95	9, 13, 25, 54	0
2	С	$66/68 \; (97\%)$	-0.11	2 (3%) 50 56	11, 19, 44, 71	0
2	D	$66/68 \; (97\%)$	-0.23	1 (1%) 73 77	12, 18, 36, 67	0
All	All	1044/1050 (99%)	-0.47	6 (0%) 89 91	9, 15, 30, 71	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	457	CYS	3.9
1	A	457	CYS	3.8
2	С	3	GLU	2.9
2	С	1	MET	2.4
1	A	388	GLY	2.2
2	D	66	GLU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	SVV	В	174	10/11	0.97	0.09	10,11,12,13	0
1	SVV	A	174	10/11	0.98	0.09	10,11,12,12	0



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	CA	A	501	1/1	0.99	0.04	17,17,17,17	0
3	CA	В	501	1/1	0.99	0.04	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.

