



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 12:11 PM BST

PDB ID : 6QMU
Title : A tetrahedral boronic acid diester formed by a non-natural amino acid in the
ligand pocket of an engineered lipocalin
Authors : Skerra, A.; Eichinger, A.
Deposited on : 2019-02-08
Resolution : 1.98 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.13.1
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)	:	2.13.1

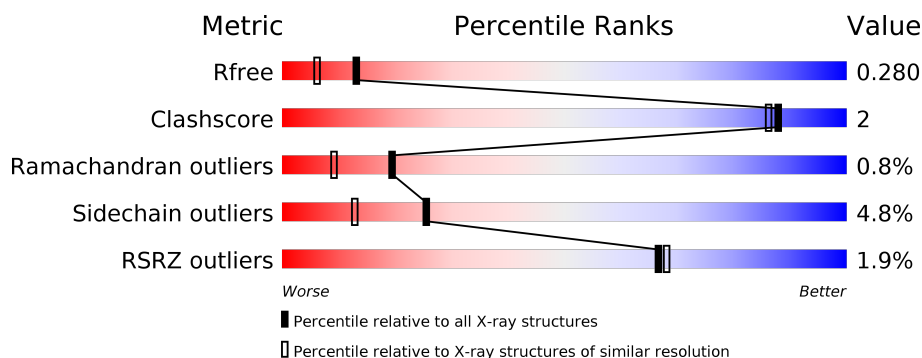
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 $\leq 5\%$. 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	188	
1	B	188	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3152 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 Neutrophil gelatinase-associated lipocalin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	184	Total	B	C	N	O	S	0	0	0
			1518	1	984	253	276	4			
1	B	184	Total	B	C	N	O	S	0	0	0
			1518	1	984	253	276	4			

There are 32 discrepancies between the modelled and reference sequences:

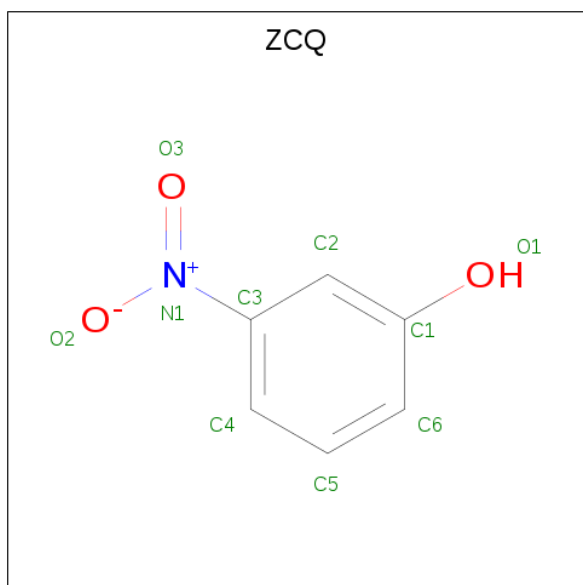
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	HIS	GLN	engineered mutation	UNP P80188
A	36	7N8	LEU	engineered mutation	UNP P80188
A	52	PHE	TYR	engineered mutation	UNP P80188
A	87	SER	CYS	engineered mutation	UNP P80188
A	125	TRP	LYS	engineered mutation	UNP P80188
A	134	ASN	LYS	engineered mutation	UNP P80188
A	179	SER	-	expression tag	UNP P80188
A	180	ALA	-	expression tag	UNP P80188
A	181	TRP	-	expression tag	UNP P80188
A	182	SER	-	expression tag	UNP P80188
A	183	HIS	-	expression tag	UNP P80188
A	184	PRO	-	expression tag	UNP P80188
A	185	GLN	-	expression tag	UNP P80188
A	186	PHE	-	expression tag	UNP P80188
A	187	GLU	-	expression tag	UNP P80188
A	188	LYS	-	expression tag	UNP P80188
B	28	HIS	GLN	engineered mutation	UNP P80188
B	36	7N8	LEU	engineered mutation	UNP P80188
B	52	PHE	TYR	engineered mutation	UNP P80188
B	87	SER	CYS	engineered mutation	UNP P80188
B	125	TRP	LYS	engineered mutation	UNP P80188
B	134	ASN	LYS	engineered mutation	UNP P80188
B	179	SER	-	expression tag	UNP P80188
B	180	ALA	-	expression tag	UNP P80188
B	181	TRP	-	expression tag	UNP P80188

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	182	SER	-	expression tag	UNP P80188
B	183	HIS	-	expression tag	UNP P80188
B	184	PRO	-	expression tag	UNP P80188
B	185	GLN	-	expression tag	UNP P80188
B	186	PHE	-	expression tag	UNP P80188
B	187	GLU	-	expression tag	UNP P80188
B	188	LYS	-	expression tag	UNP P80188

- Molecule 2 is 3-nitrophenol (three-letter code: ZCQ) (formula: $C_6H_5NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		
2	B	1	Total	C	N	O	0	0
			10	6	1	3		

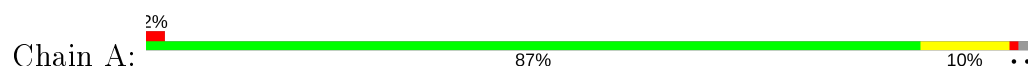
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	0
			49	49		
3	B	47	Total	O	0	0
			47	47		

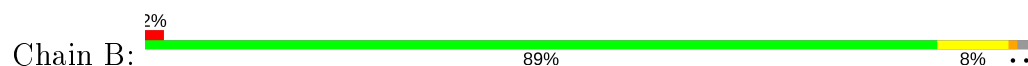
3 Residue-property plots [i](#)

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: Neutrophil gelatinase-associated lipocalin



- Molecule 1: Neutrophil gelatinase-associated lipocalin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.49Å 44.15Å 92.17Å 90.00° 133.47° 90.00°	Depositor
Resolution (Å)	66.89 – 1.98 66.89 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.1 (66.89-1.98) 97.1 (66.89-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.207 , 0.271 0.213 , 0.280	Depositor DCC
R_{free} test set	1283 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.042 for h+2*l,k,-h-l 0.023 for h,-k,-h-l 0.027 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3152	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7N8, ZCQ

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	0.49	0/1548	0.69	0/2096
1	B	0.50	0/1548	0.68	0/2096
All	All	0.50	0/3096	0.68	0/4192

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	130	ARG	Sidechain
1	B	130	ARG	Sidechain

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	1518	0	1473	6	0
1	B	1518	0	1473	6	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
3	A	49	0	0	0	0
3	B	47	0	0	0	0
All	All	3152	0	2946	12	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 2.

The worst 5 of 12 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)
1:B:120:MET:HE1	1:B:155:PHE:CD2	2.46	0.51
1:A:12:PRO:HG2	1:A:15:LYS:HG3	1.94	0.50
1:B:18:LEU:HD21	1:B:89:PRO:O	2.14	0.48
1:A:120:MET:CE	1:A:155:PHE:CD2	3.00	0.45
1:B:187:GLU:HG3	1:B:188:LYS:HE2	1.99	0.44

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	181/188 (96%)	172 (95%)	8 (4%)	1 (1%)	25	14
1	B	181/188 (96%)	174 (96%)	5 (3%)	2 (1%)	14	5
All	All	362/376 (96%)	346 (96%)	13 (4%)	3 (1%)	19	9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	SER
1	B	187	GLU
1	B	179	SER

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	167/171 (98%)	158 (95%)	9 (5%)	22	10
1	B	167/171 (98%)	160 (96%)	7 (4%)	30	17
All	All	334/342 (98%)	318 (95%)	16 (5%)	25	13

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ILE
1	A	179	SER
1	B	81	ARG
1	A	81	ARG
1	B	97	ILE

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	7N8	A	36	1,2	13,14,15	3.11	3 (23%)	15,18,20	1.38	2 (13%)
1	7N8	B	36	1,2	13,14,15	3.28	3 (23%)	15,18,20	1.84	1 (6%)

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	7N8	A	36	1,2	-	2/9/10/12	0/1/1/1
1	7N8	B	36	1,2	-	0/9/10/12	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	7N8	BZ-OB2	9.24	1.52	1.36
1	B	36	7N8	BZ-OB2	8.91	1.51	1.36
1	B	36	7N8	BZ-OB1	7.28	1.48	1.36
1	A	36	7N8	BZ-OB1	5.75	1.46	1.36
1	A	36	7N8	BZ-CZ	2.13	1.61	1.57

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	7N8	OB2-BZ-CZ	-6.10	101.72	119.95
1	A	36	7N8	OB2-BZ-OB1	-3.32	108.50	119.67
1	A	36	7N8	OB2-BZ-CZ	-2.86	111.41	119.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	36	7N8	OB2-BZ-CZ-CE2
1	A	36	7N8	OB2-BZ-CZ-CE1

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](#)

2 ligands 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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ZCQ	A	201	1	9,10,10	0.37	0	11,13,13	1.99	4 (36%)
2	ZCQ	B	201	1	9,10,10	0.32	0	11,13,13	1.88	3 (27%)

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
2	ZCQ	A	201	1	-	0/2/4/4	0/1/1/1
2	ZCQ	B	201	1	-	0/2/4/4	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	ZCQ	O1-C1-C6	-3.51	110.02	120.02
2	B	201	ZCQ	O1-C1-C6	-3.47	110.13	120.02
2	A	201	ZCQ	O1-C1-C2	3.41	128.69	119.84
2	B	201	ZCQ	O1-C1-C2	3.36	128.58	119.84
2	A	201	ZCQ	C4-C3-C2	2.50	123.26	120.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	ZCQ	1	0

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	183/188 (97%)	0.07	3 (1%) 72 73	23, 34, 53, 79	0
1	B	183/188 (97%)	0.22	4 (2%) 62 63	22, 36, 58, 88	0
All	All	366/376 (97%)	0.15	7 (1%) 66 68	22, 35, 55, 88	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	SER	3.6
1	B	185	GLN	3.4
1	B	188	LYS	3.3
1	B	5	SER	2.9
1	B	186	PHE	2.6

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, 95th 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	B-factors(Å ²)	Q<0.9
1	7N8	B	36	14/15	0.81	0.15	26,38,43,44	0
1	7N8	A	36	14/15	0.94	0.11	22,28,31,32	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, 95th 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	B-factors(\AA^2)	Q<0.9
2	ZCQ	B	201	10/10	0.88	0.19	44,49,61,63	0
2	ZCQ	A	201	10/10	0.91	0.14	31,33,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.