wwPDB X-ray Structure Validation Summary Report (i)

Sep 12, 2023 – 12:23 AM EDT

PDB ID	:	4MVK
Title	:	Crystal structure of an engineered lipocalin (Anticalin US7) in complex with the Alzheimer amyloid peptide fragment VFFAED
Authors	:	Eichinger, A.; Skerra, A.
Deposited on	:	2013-09-24
Resolution	:	1.50 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 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:

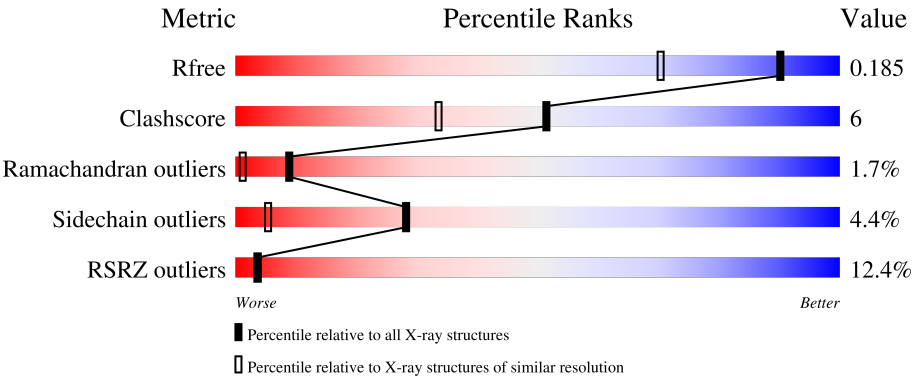
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	188	12% 77% 10% • 9%
2	B	8	88% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1598 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	171	Total	C	N	O	S	0	0	0
			1386	891	242	249	4			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	HIS	GLN	engineered mutation	UNP P80188
A	36	VAL	LEU	engineered mutation	UNP P80188
A	40	LYS	ALA	engineered mutation	UNP P80188
A	41	SER	ILE	engineered mutation	UNP P80188
A	49	TRP	GLN	engineered mutation	UNP P80188
A	70	GLY	LEU	engineered mutation	UNP P80188
A	72	GLY	ARG	engineered mutation	UNP P80188
A	73	THR	LYS	engineered mutation	UNP P80188
A	77	HIS	ASP	engineered mutation	UNP P80188
A	79	LYS	TRP	engineered mutation	UNP P80188
A	87	SER	CYS	engineered mutation	UNP P80188
A	96	ARG	ASN	engineered mutation	UNP P80188
A	100	ARG	TYR	engineered mutation	UNP P80188
A	103	ARG	LEU	engineered mutation	UNP P80188
A	106	ALA	TYR	engineered mutation	UNP P80188
A	125	VAL	LYS	engineered mutation	UNP P80188
A	127	GLN	SER	engineered mutation	UNP P80188
A	132	SER	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	187	GLU	-	expression tag	UNP P80188
A	188	LYS	-	expression tag	UNP P80188

- Molecule 2 is a protein called Amyloid peptide fragment VFFAED.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	8	Total C N O 55 37 7 11	0	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	ACE	-	expression tag	UNP P05067
B	24	NH2	-	expression tag	UNP P05067

- Molecule 3 is water.

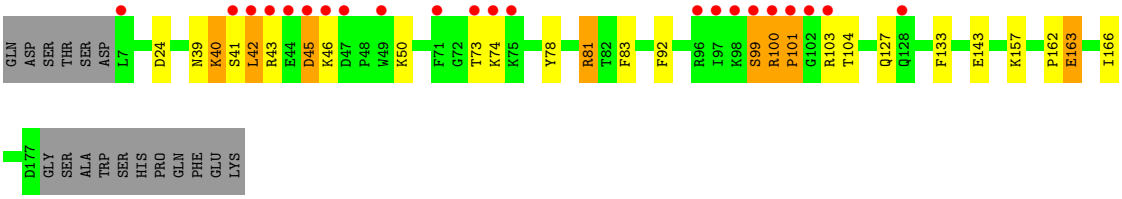
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	148	Total O 148 148	0	0
3	B	9	Total O 9 9	0	0

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: Neutrophil gelatinase-associated lipocalin

Chain A:



• Molecule 2: Amyloid peptide fragment VFFAED

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.97Å 59.23Å 61.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.57 – 1.50 26.66 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.57-1.50) 99.6 (26.66-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.04 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.165 , 0.186 0.164 , 0.185	Depositor DCC
R_{free} test set	1530 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.785	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 58.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	1598	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.39% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, NH2

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	1.15	2/1422 (0.1%)	1.11	5/1923 (0.3%)
2	B	1.29	0/53	1.32	1/71 (1.4%)
All	All	1.15	2/1475 (0.1%)	1.11	6/1994 (0.3%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	GLU	CD-OE2	-6.27	1.18	1.25
1	A	81	ARG	CZ-NH1	5.95	1.40	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	81	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	92	PHE	CB-CG-CD1	-6.04	116.57	120.80
1	A	24	ASP	CB-CG-OD1	6.04	123.73	118.30
1	A	45	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	83	PHE	CB-CG-CD2	-5.51	116.94	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	LYS	Peptide

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	1386	0	1388	16	0
2	B	55	0	45	0	0
3	A	148	0	0	1	0
3	B	9	0	0	0	0
All	All	1598	0	1433	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 6.

The worst 5 of 16 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:A:100:ARG:CB	1:A:101:PRO:HD2	2.20	0.71
1:A:163:GLU:HA	1:A:166:ILE:HD12	1.75	0.67
1:A:43:ARG:HH21	1:A:45:ASP:HB3	1.62	0.64
1:A:104:THR:HG23	1:A:127:GLN:HG2	1.81	0.62
1:A:100:ARG:HB3	1:A:101:PRO:HD2	1.89	0.54

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	169/188 (90%)	157 (93%)	9 (5%)	3 (2%)	8 1
2	B	6/8 (75%)	4 (67%)	2 (33%)	0	100 100
All	All	175/196 (89%)	161 (92%)	11 (6%)	3 (2%)	9 1

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	101	PRO
1	A	99	SER

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	155/170 (91%)	148 (96%)	7 (4%)	27 5
2	B	5/5 (100%)	5 (100%)	0	100 100
All	All	160/175 (91%)	153 (96%)	7 (4%)	28 5

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	103	ARG
1	A	163	GLU
1	A	162	PRO
1	A	99	SER

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)

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

6.1 Protein, DNA and RNA chains

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>2	OWAB(Å^2)	Q<0.9
1	A	171/188 (90%)	0.72	22 (12%) 3 3	9, 17, 62, 111	0
2	B	6/8 (75%)	-0.37	0 100 100	11, 14, 16, 20	0
All	All	177/196 (90%)	0.69	22 (12%) 4 3	9, 17, 62, 111	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	GLY	10.0
1	A	101	PRO	9.0
1	A	42	LEU	8.0
1	A	97	ILE	7.2
1	A	100	ARG	7.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.