

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 10, 2021 – 07:38 PM EDT

PDB ID	:	3GI8
Title	:	Crystal Structure of ApcT K158A Transporter Bound to 7F11 Monoclonal Fab
		Fragment
Authors	:	Shaffer, P.L.; Goehring, A.S.; Shankaranarayanan, A.; Gouaux, E.; New York
		Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on	:	2009-03-05
Resolution	:	2.59  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 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	:	2.23.2
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)	:	2.23.2

# 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 2.59 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	С	444	88%	10%	·
2	L	220	83%	15%	•
3	Н	223	4%	10%	



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6924 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 Uncharacterized protein MJ0609.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	С	435	Total 3351	C 2261	N 512	O 567	S 11	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	158	ALA	LYS	engineered mutation	UNP Q58026
С	436	LEU	-	expression tag	UNP Q58026
С	437	GLU	-	expression tag	UNP Q58026
С	438	SER	-	expression tag	UNP Q58026
С	439	SER	-	expression tag	UNP Q58026
С	440	GLY	-	expression tag	UNP Q58026
С	441	LEU	-	expression tag	UNP Q58026
С	442	VAL	-	expression tag	UNP Q58026
С	443	PRO	-	expression tag	UNP Q58026
С	444	ARG	-	expression tag	UNP Q58026

• Molecule 2 is a protein called 7F11 Anti-ApcT Monoclonal Fab Light Chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	L	220	Total	С	N	0	S	0	0	0
		_	1705	1061	285	351	8	_	_	-

• Molecule 3 is a protein called 7F11 Anti-ApcT Monoclonal Fab Heavy Chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	Н	220	Total 1664	C 1057	N 264	0 334	S 9	0	0	0

• Molecule 4 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	57	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 57 & 57 \end{array}$	0	0
4	L	76	Total         O           76         76	0	0
4	Н	71	Total         O           71         71	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: Uncharacterized protein MJ0609



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	46.04Å 111.19Å 115.67Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.92^{\circ}$ $90.00^{\circ}$	Depositor
<b>D</b> ecolution $(\hat{A})$	50.00 - 2.59	Depositor
Resolution (A)	40.11 - 2.59	EDS
% Data completeness	99.6 (50.00-2.59)	Depositor
(in resolution range)	99.6 (40.11-2.59)	EDS
R <sub>merge</sub>	0.09	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.47 (at 2.58 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
P. P.	0.254 , $0.307$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.252 , $0.307$	DCC
$R_{free}$ test set	1805 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	47.9	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29, $44.9$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.33$	Xtriage
	0.000 for -h,l,k	
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
	0.029 for h,-k,-l	
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6924	wwPDB-VP
Average B, all atoms $(Å^2)$	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities 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).

Mal	Chain	Bond	lengths	Bond angles		
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	С	0.36	0/3432	0.44	0/4660	
2	L	0.35	0/1742	0.53	0/2361	
3	Н	0.34	0/1713	0.50	0/2345	
All	All	0.35	0/6887	0.48	0/9366	

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	С	3351	0	3510	29	0
2	L	1705	0	1635	20	0
3	Н	1664	0	1592	10	0
4	С	57	0	0	2	0
4	Н	71	0	0	0	0
4	L	76	0	0	1	0
All	All	6924	0	6737	59	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 4.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:425:ARG:HH11	1:C:425:ARG:HG2	1.38	0.87
2:L:216:ASN:HB2	2:L:219:GLU:HG3	1.59	0.81
3:H:70:LEU:HD21	3:H:81:MET:HE3	1.68	0.75
2:L:216:ASN:HB2	2:L:219:GLU:CG	2.21	0.70
2:L:13:MET:HG3	2:L:19:VAL:HG22	1.72	0.70
1:C:121:ASN:HB2	1:C:124:ASN:H	1.57	0.68
1:C:434:LYS:HB3	1:C:435:SER:HA	1.77	0.66
3:H:102:TYR:O	3:H:105:THR:HG22	1.96	0.66
2:L:43:GLN:HB2	2:L:53:LEU:HD11	1.82	0.61
2:L:31:ASN:O	2:L:35:GLN:HA	2.00	0.60
2:L:131:LEU:O	2:L:189:LYS:HE3	2.02	0.60
1:C:433:VAL:HG12	1:C:434:LYS:O	2.02	0.59
1:C:425:ARG:HH11	1:C:425:ARG:CG	2.14	0.58
1:C:268:LEU:HB3	1:C:272:GLY:HA3	1.84	0.58
2:L:131:LEU:C	2:L:133:SER:H	2.11	0.53
1:C:433:VAL:O	1:C:434:LYS:HB2	2.08	0.53
3:H:105:THR:HG23	3:H:107:TYR:H	1.74	0.52
1:C:270:ASN:HA	1:C:273:PHE:HB3	1.91	0.51
1:C:97:TYR:HD1	1:C:291:THR:HG23	1.77	0.50
2:L:151:ASN:HB3	2:L:203:THR:HB	1.95	0.49
1:C:97:TYR:OH	1:C:209:ASN:ND2	2.40	0.49
3:H:203:THR:HG23	3:H:220:LYS:HE3	1.96	0.48
1:C:98:VAL:HG22	1:C:327:THR:HG23	1.96	0.47
1:C:304:LYS:O	1:C:425:ARG:HD3	2.16	0.46
1:C:140:ASN:HB2	1:C:293:TYR:OH	2.15	0.46
1:C:183:ALA:HA	1:C:184:PRO:HD3	1.87	0.45
2:L:37:ASN:HD21	2:L:74:GLY:H	1.63	0.45
3:H:159:GLU:HA	3:H:160:SER:HA	1.75	0.45
2:L:127:SER:C	2:L:129:GLU:H	2.20	0.44
3:H:68:ALA:HB1	3:H:81:MET:HE2	2.00	0.44
2:L:118:ALA:HA	2:L:206:THR:HG21	1.99	0.44
1:C:414:ILE:HA	4:C:488:HOH:O	2.17	0.44
1:C:71:GLY:HA3	1:C:72:PRO:HD2	1.85	0.43
1:C:76:ILE:HD13	1:C:89:LEU:HD13	1.99	0.43
2:L:153:LYS:HB2	2:L:201:GLU:HB2	2.01	0.43
2:L:156:ILE:HD11	2:L:185:LEU:HD21	2.01	0.43
3:H:155:GLY:HA2	3:H:185:LEU:HB3	1.99	0.43
2:L:124:PHE:HA	2:L:125:PRO:HD3	1.92	0.42
3:H:38:LYS:HB2	3:H:48:ILE:HD11	2.00	0.42
2:L:87:GLU:H	2:L:87:GLU:HG3	1.71	0.42
1:C:379:SER:HB2	4:C:490:HOH:O	2.19	0.42
3:H:50:GLU:HG2	3:H:59:ASN:HB3	2.02	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:46:ILE:O	1:C:50:ILE:HG12	2.19	0.42
1:C:221:VAL:HB	1:C:222:PRO:HD3	2.02	0.42
2:L:201:GLU:HG2	2:L:212:VAL:HG22	2.00	0.42
1:C:60:THR:HG22	1:C:222:PRO:HA	2.01	0.41
1:C:373:LYS:O	1:C:377:ILE:HG13	2.20	0.41
2:L:34:ASN:HB2	4:L:288:HOH:O	2.20	0.41
2:L:38:TYR:CD2	2:L:38:TYR:N	2.88	0.41
1:C:211:SER:HB2	1:C:221:VAL:HG21	2.02	0.41
1:C:434:LYS:CB	1:C:435:SER:HA	2.46	0.41
1:C:62:LEU:HD23	1:C:369:VAL:HG11	2.03	0.41
2:L:37:ASN:ND2	2:L:74:GLY:H	2.19	0.41
1:C:410:ILE:O	1:C:414:ILE:HG12	2.20	0.41
1:C:425:ARG:HG2	1:C:425:ARG:NH1	2.18	0.41
2:L:204:HIS:HB3	2:L:206:THR:HG22	2.02	0.41
3:H:48:ILE:HG21	3:H:81:MET:CE	2.51	0.41
1:C:228:SER:O	1:C:232:VAL:HG22	2.21	0.40
1:C:184:PRO:HA	1:C:187:VAL:HB	2.02	0.40

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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	С	433/444~(98%)	414 (96%)	19 (4%)	0	100 100
2	L	218/220~(99%)	204 (94%)	11 (5%)	3~(1%)	11 22
3	Н	216/223~(97%)	210 (97%)	6 (3%)	0	100 100
All	All	867/887~(98%)	828 (96%)	36~(4%)	3~(0%)	41 64

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	L	132	THR
2	L	128	SER
2	L	74	GLY

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
1	С	352/360~(98%)	345~(98%)	7~(2%)	55	78
2	L	198/198~(100%)	189~(96%)	9 (4%)	27	52
3	Н	191/194 (98%)	182 (95%)	9~(5%)	26	50
All	All	741/752~(98%)	716 (97%)	25 (3%)	37	63

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	6	LYS
1	С	198	PHE
1	С	226	PHE
1	С	246	ASN
1	С	307	GLU
1	С	399	ARG
1	С	425	ARG
2	L	38	TYR
2	L	39	LEU
2	L	84	VAL
2	L	85	GLN
2	L	87	GLU
2	L	129	GLU
2	L	132	THR
2	L	187	LEU
2	L	193	GLU
3	Н	5	LEU
3	Н	12	VAL
3	Н	89	GLN
3	Н	102	TYR



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Mol	Chain	Res	Type
3	Н	106	THR
3	Н	127	THR
3	Н	139	CYS
3	Н	143	THR
3	Н	189	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	С	5	ASN
1	С	209	ASN
1	С	246	ASN
1	С	394	GLN
1	С	430	ASN
2	L	27	GLN
2	L	37	ASN
2	L	143	ASN
2	L	144	ASN
2	L	162	GLN
2	L	163	ASN
2	L	167	ASN
3	Н	62	GLN
3	Н	175	HIS

#### 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,  $95^{th}$  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	С	435/444~(97%)	1.10	88 (20%) 1 0	36, 71, 101, 104	0
2	L	220/220~(100%)	-0.04	3 (1%) 75 71	28, 41, 54, 68	0
3	Н	220/223~(98%)	0.12	8 (3%) 42 35	29,  43,  64,  67	0
All	All	875/887~(98%)	0.57	99 (11%) 5 3	28, 53, 96, 104	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	220	CYS	8.7
1	С	168	ALA	8.3
1	С	127	ILE	8.0
1	С	278	ILE	6.5
1	С	271	LEU	6.1
1	С	392	TYR	5.4
2	L	100	THR	4.9
1	С	267	PHE	4.7
1	С	124	ASN	4.6
1	С	396	ILE	4.5
1	С	39	ARG	4.4
1	С	167	PHE	4.2
1	С	177	TYR	4.2
1	С	182	LEU	4.1
1	С	142	PHE	4.1
3	Н	139	CYS	4.0
1	С	125	ILE	3.9
1	С	250	ASP	3.9
1	С	259	ALA	3.8
1	С	244	ILE	3.8
1	С	172	THR	3.8
1	С	414	ILE	3.7
1	C	117	ASN	3.6



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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
1         C         123         PHE         3.4           1         C         31         GLY         3.3           1         C         256         SER         3.3           1         C         368         GLU         3.2           1         C         262         VAL         3.2           1         C         410         ILE         3.2           1         C         420         VAL         3.2           1         C         410         ILE         3.2           1         C         102         PHE         3.1	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
1         C         256         SER         3.3           1         C         368         GLU         3.2           1         C         262         VAL         3.2           1         C         410         ILE         3.2           1         C         410         ILE         3.1           1         C         192         PHE         3.1	
1         C         368         GLU         3.2           1         C         262         VAL         3.2           1         C         410         ILE         3.2           1         C         22         ILE         3.1           1         C         192         PHE         3.1	
1         C         262         VAL         3.2           1         C         410         ILE         3.2           1         C         22         ILE         3.1           1         C         192         PHE         3.1	
1         C         410         ILE         3.2           1         C         22         ILE         3.1           1         C         192         PHE         3.1	
1         C         22         ILE         3.1           1         C         192         PHE         3.1	
1 C 192 PHE 3.1	
1 C 35 LYS 3.0	
1 C 274 LEU 3.0	
1 C 284 ILE 3.0	
1 C 21 MET 2.9	
1 C 112 PHE 2.9	
3 H 167 SER 2.9	
1 C 234 PHE 2.9	
1 C 17 ALA 2.8	
1 C 186 ALA 2.8	
1 C 258 ASN 2.8	
1 C 116 ILE 2.8	
1 C 100 SER 2.8	
1 C 340 MET 2.8	
1 C 276 ILE 2.8	
1 C 115 LEU 2.7	
3 H 138 GLY 2.7	
1 C 226 PHE 2.7	
1 C 266 PRO 2.7	
1 C 434 LYS 2.7	
3         H         169         SER         2.6	I
3         H         169         SER         2.6           1         C         128         THR         2.6	_
3         H         169         SER         2.6           1         C         128         THR         2.6           1         C         26         ILE         2.6	_
3         H         169         SER         2.6           1         C         128         THR         2.6           1         C         26         ILE         2.6           1         C         26         ILE         2.6           1         C         170         LEU         2.6	
3         H         169         SER         2.6           1         C         128         THR         2.6           1         C         26         ILE         2.6           1         C         26         ILE         2.6           1         C         170         LEU         2.6           1         C         183         ALA         2.6	
3         H         169         SER         2.6           1         C         128         THR         2.6           1         C         26         ILE         2.6           1         C         170         LEU         2.6           1         C         170         LEU         2.6           1         C         183         ALA         2.6           3         H         170         LEU         2.5	



Mol	Chain	Res	Type	RSRZ
1	С	257	GLU	2.5
1	С	397	THR	2.5
1	С	253	ILE	2.4
1	С	23	GLY	2.4
1	С	400	PHE	2.4
2	L	218	ASN	2.4
1	С	336	LEU	2.4
1	С	175	PRO	2.4
1	С	20	VAL	2.4
3	Н	26	GLY	2.4
1	С	108	PHE	2.4
1	С	179	ILE	2.4
1	С	247	LEU	2.4
1	С	249	ILE	2.3
1	С	287	ALA	2.3
1	С	275	LEU	2.3
1	С	206	VAL	2.3
1	С	203	GLY	2.3
1	С	233	MET	2.2
3	Н	214	SER	2.2
1	С	395	TRP	2.2
1	С	36	ILE	2.2
1	С	245	GLY	2.2
1	С	164	LEU	2.2
1	С	391	LEU	2.2
1	С	18	VAL	2.1
1	С	293	TYR	2.1
1	С	219	LYS	2.1
1	С	110	GLY	2.1
1	С	171	ILE	2.0
1	С	231	ILE	2.0
1	С	103	LEU	2.0
1	С	252	LEU	2.0
1	С	96	SER	2.0

Continued from previous page...

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

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

3GI8



### 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.

