Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:48 pm BST

PDB ID	:	3GI9
Title	:	Crystal Structure of ApcT 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	:	2.48 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 ⓘ symbol.

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

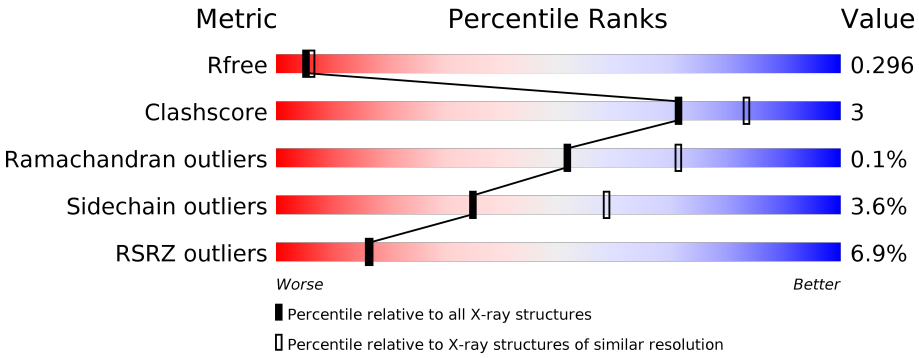
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.48 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	L	220	7% 84% 14%
2	H	223	4% 86% 10%
3	C	444	8% 91% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6865 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 7F11 Anti-ApcT Monoclonal Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	219	Total	C	N	O	S	0	0	0
			1698	1058	284	349	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1646	1048	261	329	8			

- Molecule 3 is a protein called Uncharacterized protein MJ0609.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	437	Total	C	N	O	S	0	0	0
			3370	2274	514	571	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	436	LEU	-	EXPRESSION TAG	UNP Q58026
C	437	GLU	-	EXPRESSION TAG	UNP Q58026
C	438	SER	-	EXPRESSION TAG	UNP Q58026
C	439	SER	-	EXPRESSION TAG	UNP Q58026
C	440	GLY	-	EXPRESSION TAG	UNP Q58026
C	441	LEU	-	EXPRESSION TAG	UNP Q58026
C	442	VAL	-	EXPRESSION TAG	UNP Q58026
C	443	PRO	-	EXPRESSION TAG	UNP Q58026
C	444	ARG	-	EXPRESSION TAG	UNP Q58026

- Molecule 4 is water.

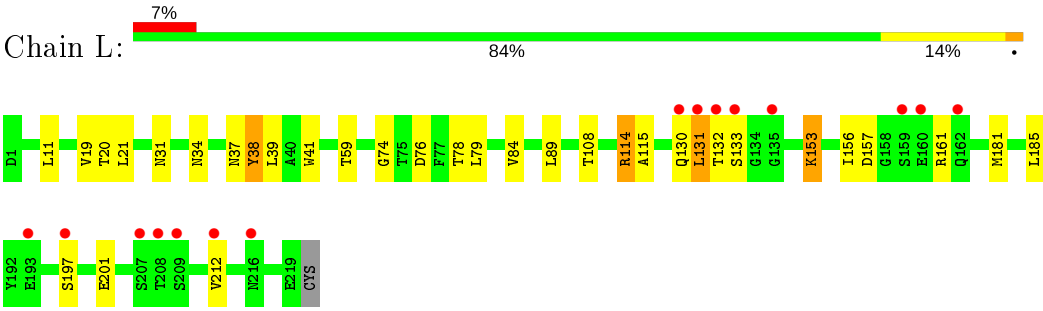
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	53	Total O 53 53	0	0
4	H	60	Total O 60 60	0	0
4	C	38	Total O 38 38	0	0

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.

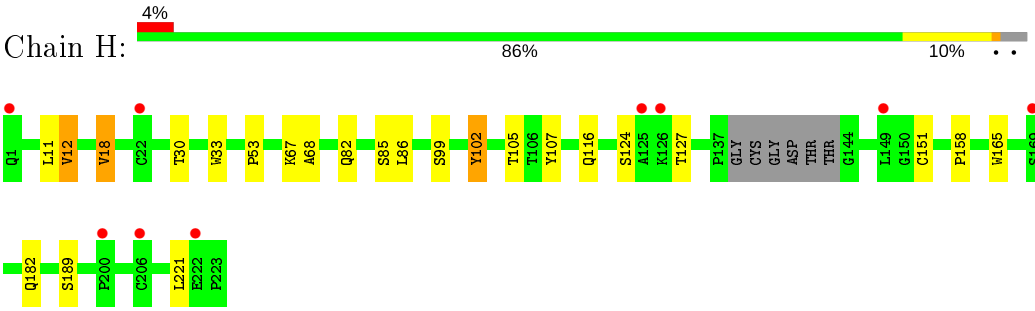
- Molecule 1: 7F11 Anti-ApcT Monoclonal Fab Light Chain

Chain L:



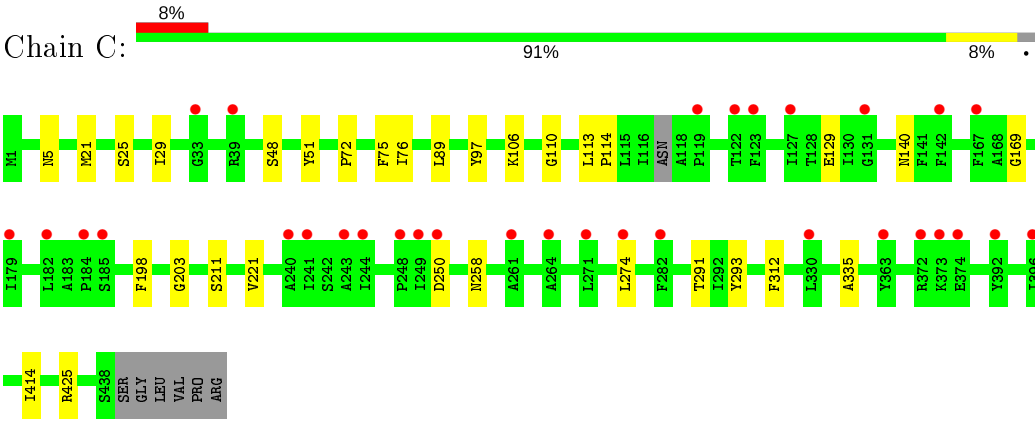
- Molecule 2: 7F11 Anti-ApcT Monoclonal Fab Heavy Chain

Chain H:



- Molecule 3: Uncharacterized protein MJ0609

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.37Å 45.90Å 158.09Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	50.00 – 2.48 43.81 – 2.48	Depositor EDS
% Data completeness (in resolution range)	94.1 (50.00-2.48) 94.1 (43.81-2.48)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.296 0.247 , 0.296	Depositor DCC
R_{free} test set	1819 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	45.8	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 35.8	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	0.91	EDS
Total number of atoms	6865	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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

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	L	0.34	0/1735	0.52	0/2353
2	H	0.34	0/1695	0.51	0/2322
3	C	0.35	0/3450	0.44	0/4681
All	All	0.35	0/6880	0.48	0/9356

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

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	L	1698	0	1631	17	0
2	H	1646	0	1578	11	0
3	C	3370	0	3533	19	0
4	C	38	0	0	2	0
4	H	60	0	0	1	0
4	L	53	0	0	1	0
All	All	6865	0	6742	47	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.

All (47) 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)
3:C:425:ARG:HG2	3:C:425:ARG:HH11	1.46	0.81
2:H:12:VAL:HG11	2:H:18:VAL:HG13	1.74	0.69
2:H:105:THR:HG23	2:H:107:TYR:H	1.57	0.68
3:C:113:LEU:HD11	4:C:481:HOH:O	1.97	0.63
1:L:31:ASN:HB3	1:L:34:ASN:HB2	1.80	0.62
1:L:37:ASN:HD21	1:L:74:GLY:H	1.48	0.61
1:L:20:THR:HG23	1:L:78:THR:HG23	1.82	0.60
1:L:157:ASP:HA	1:L:197:SER:HB3	1.84	0.59
2:H:102:TYR:O	2:H:105:THR:HG22	2.03	0.59
3:C:5:ASN:HD21	3:C:312:PHE:H	1.52	0.57
3:C:106:LYS:HG3	3:C:129:GLU:OE2	2.04	0.56
1:L:21:LEU:HD22	1:L:108:THR:HG21	1.88	0.54
3:C:76:ILE:HD13	3:C:89:LEU:HD13	1.88	0.54
3:C:113:LEU:HB2	3:C:114:PRO:HD3	1.91	0.53
3:C:140:ASN:HB2	3:C:293:TYR:OH	2.11	0.51
3:C:425:ARG:HH11	3:C:425:ARG:CG	2.21	0.50
1:L:114:ARG:HD3	1:L:115:ALA:O	2.12	0.50
3:C:106:LYS:NZ	3:C:335:ALA:O	2.46	0.49
3:C:110:GLY:O	3:C:258:ASN:HB3	2.13	0.48
1:L:37:ASN:ND2	1:L:74:GLY:H	2.11	0.47
3:C:21:MET:HE3	3:C:203:GLY:H	1.80	0.47
3:C:211:SER:HB2	3:C:221:VAL:HG21	1.98	0.45
2:H:18:VAL:HG22	2:H:86:LEU:HD11	1.98	0.45
3:C:97:TYR:HD1	3:C:291:THR:HG23	1.82	0.44
1:L:201:GLU:HG2	1:L:212:VAL:HG22	1.98	0.44
2:H:33:TRP:HB2	2:H:99:SER:HB3	1.99	0.44
3:C:25:SER:HA	3:C:29:ILE:HG12	1.98	0.44
2:H:116:GLN:HB2	4:H:226:HOH:O	2.18	0.44
1:L:20:THR:HG23	1:L:78:THR:CG2	2.47	0.43
1:L:131:LEU:HD12	1:L:132:THR:HG23	2.01	0.42
3:C:72:PRO:HA	3:C:75:PHE:CD2	2.54	0.42
1:L:38:TYR:N	1:L:38:TYR:CD2	2.87	0.42
2:H:165:TRP:HZ3	2:H:221:LEU:CD1	2.31	0.42
1:L:59:THR:HG23	4:L:236:HOH:O	2.19	0.42
2:H:30:THR:HA	2:H:53:PRO:HB2	2.01	0.42
1:L:156:ILE:HD11	1:L:185:LEU:HD21	2.01	0.42
1:L:131:LEU:O	1:L:189:LYS:HD3	2.20	0.42
1:L:131:LEU:C	1:L:133:SER:H	2.23	0.41
1:L:41:TRP:CE2	1:L:79:LEU:HB2	2.55	0.41
1:L:153:LYS:HB2	1:L:201:GLU:HB2	2.02	0.41
2:H:11:LEU:HB2	2:H:158:PRO:HG3	2.03	0.41
2:H:68:ALA:HA	2:H:82:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:410:ILE:O	3:C:414:ILE:HG12	2.19	0.41
3:C:48:SER:HA	3:C:51:TYR:CD2	2.55	0.41
3:C:113:LEU:CD1	4:C:481:HOH:O	2.64	0.41
3:C:169:GLY:O	3:C:173:ILE:HG23	2.21	0.40
2:H:177:PHE:HA	2:H:178:PRO:HD3	1.87	0.40

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	L	217/220 (99%)	206 (95%)	11 (5%)	0	100 100
2	H	213/223 (96%)	202 (95%)	10 (5%)	1 (0%)	29 46
3	C	433/444 (98%)	420 (97%)	13 (3%)	0	100 100
All	All	863/887 (97%)	828 (96%)	34 (4%)	1 (0%)	51 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	85	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	L	197/198 (100%)	183 (93%)	14 (7%)	14 26
2	H	189/194 (97%)	180 (95%)	9 (5%)	25 45
3	C	355/361 (98%)	351 (99%)	4 (1%)	73 88
All	All	741/753 (98%)	714 (96%)	27 (4%)	35 58

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	11	LEU
1	L	19	VAL
1	L	38	TYR
1	L	39	LEU
1	L	76	ASP
1	L	84	VAL
1	L	89	LEU
1	L	114	ARG
1	L	130	GLN
1	L	131	LEU
1	L	153	LYS
1	L	161	ARG
1	L	181	MET
1	L	191	GLU
2	H	12	VAL
2	H	18	VAL
2	H	67	LYS
2	H	102	TYR
2	H	124	SER
2	H	127	THR
2	H	151	CYS
2	H	182	GLN
2	H	189	SER
3	C	177	TYR
3	C	198	PHE
3	C	250	ASP
3	C	274	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	37	ASN
1	L	85	GLN

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Mol	Chain	Res	Type
1	L	143	ASN
1	L	144	ASN
2	H	1	GLN
2	H	62	GLN
2	H	116	GLN
3	C	5	ASN
3	C	209	ASN
3	C	289	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	L	219/220 (99%)	0.27	15 (6%)	17	17	28, 42, 66, 75	0
2	H	217/223 (97%)	0.08	10 (4%)	32	34	27, 38, 54, 57	3 (1%)
3	C	437/444 (98%)	0.58	35 (8%)	12	11	34, 59, 87, 90	0
All	All	873/887 (98%)	0.38	60 (6%)	16	16	27, 49, 84, 90	3 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	184	PRO	8.0
3	C	182	LEU	5.9
3	C	244	ILE	5.6
3	C	271	LEU	5.5
1	L	212	VAL	5.4
3	C	142	PHE	5.4
3	C	400	PHE	5.4
3	C	392	TYR	4.8
3	C	178	VAL	4.6
2	H	125	ALA	4.2
2	H	170	LEU	4.0
3	C	127	ILE	3.8
2	H	22	CYS	3.8
2	H	206	CYS	3.6
2	H	126	LYS	3.5
3	C	249	ILE	3.5
3	C	241	ILE	3.4
1	L	209	SER	3.4
2	H	200	PRO	3.4
1	L	131	LEU	3.3
1	L	130	GLN	3.3
1	L	208	THR	3.3
3	C	123	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	169	SER	3.2
3	C	363	TYR	3.2
3	C	282	PHE	3.2
1	L	132	THR	3.2
3	C	373	LYS	3.0
3	C	274	LEU	3.0
3	C	39	ARG	3.0
3	C	119	PRO	3.0
3	C	240	ALA	2.9
3	C	261	ALA	2.9
3	C	131	GLY	2.8
1	L	207	SER	2.8
3	C	185	SER	2.8
1	L	133	SER	2.8
3	C	33	GLY	2.6
3	C	374	GLU	2.6
1	L	135	GLY	2.5
3	C	250	ASP	2.5
3	C	372	ARG	2.4
3	C	396	ILE	2.4
3	C	179	ILE	2.3
2	H	149	LEU	2.3
3	C	330	LEU	2.3
3	C	243	ALA	2.3
3	C	177	TYR	2.3
1	L	159	SER	2.2
1	L	216	ASN	2.2
1	L	197	SER	2.2
1	L	193	GLU	2.1
3	C	167	PHE	2.1
2	H	1	GLN	2.1
3	C	248	PRO	2.1
1	L	160	GLU	2.1
2	H	222	GLU	2.0
3	C	122	THR	2.0
1	L	162	GLN	2.0
3	C	264	ALA	2.0

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

There are no carbohydrates 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.