



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:06 am GMT

PDB ID : 4ZD3
Title : Structure of a transglutaminase 2-specific autoantibody Fab fragment
Authors : Chen, X.; Dalhus, B.; Hnida, K.; Iversen, R.; Sollid, L.M.
Deposited on : 2015-04-16
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

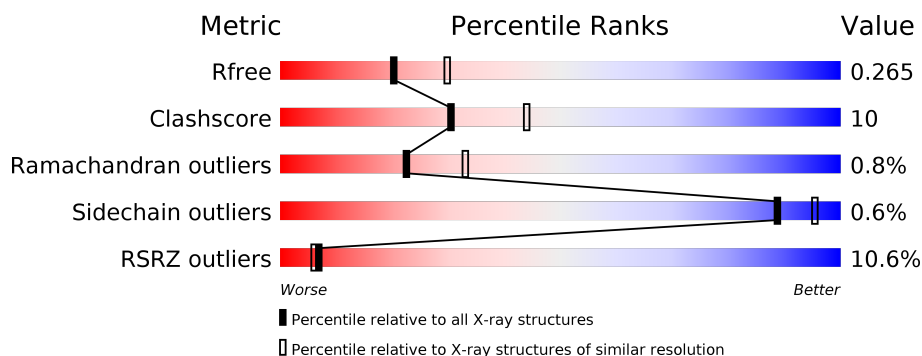
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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. 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	H	224	
2	L	216	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3175 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 679-14-14E06 Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	199	Total	C	N	O	S	0	0	0
			1518	972	244	294	8			

- Molecule 2 is a protein called 679-14-14E06 Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	205	Total	C	N	O	S	0	0	0
			1579	991	262	321	5			

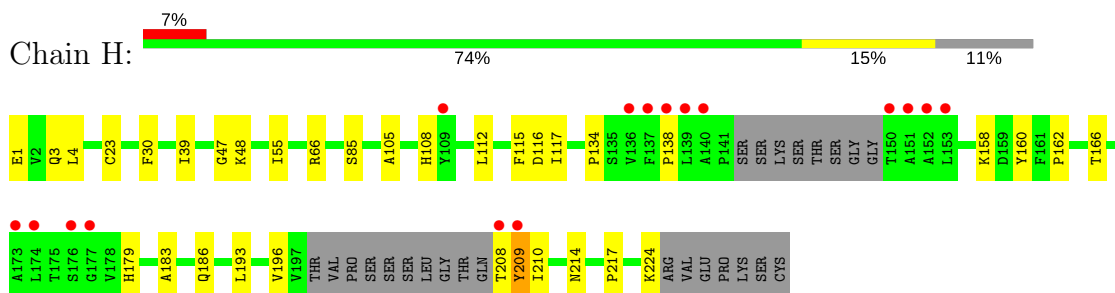
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	53	Total	O	0	0
			53	53		
3	L	25	Total	O	0	0
			25	25		

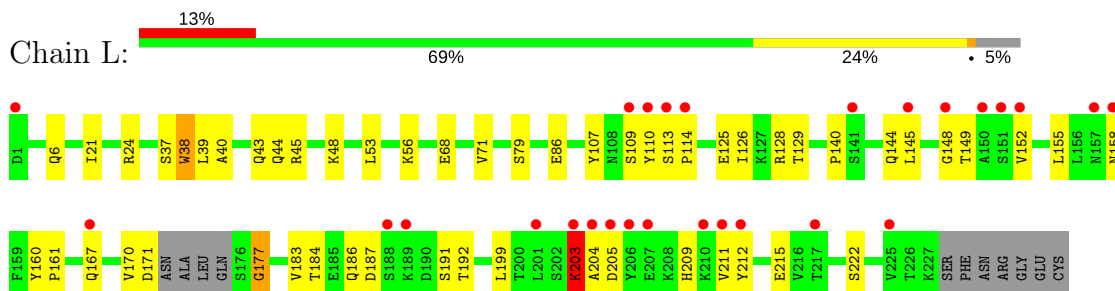
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: 679-14-14E06 Fab fragment heavy chain



- Molecule 2: 679-14-14E06 Fab fragment light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.34Å 61.38Å 79.05Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	49.43 – 2.40 49.43 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.43-2.40) 94.4 (49.43-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.200 , 0.264 0.203 , 0.265	Depositor DCC
R_{free} test set	943 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3175	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	H	0.44	0/1560	0.58	0/2124
2	L	0.49	0/1615	0.69	2/2193 (0.1%)
All	All	0.47	0/3175	0.64	2/4317 (0.0%)

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	H	0	1
2	L	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	L	205	ASP	N-CA-C	-5.92	95.02	111.00
2	L	205	ASP	CB-CA-C	5.14	120.67	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	209	TYR	Peptide
2	L	203	LYS	Peptide
2	L	204	ALA	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	H	1518	0	1471	24	0
2	L	1579	0	1530	44	0
3	H	53	0	0	3	0
3	L	25	0	0	9	0
All	All	3175	0	3001	64	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 10.

All (64) 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:H:66:ARG:HG3	2:L:114:PRO:HG2	1.47	0.94
1:H:108:HIS:NE2	3:H:301:HOH:O	2.13	0.74
1:H:208:THR:HG22	1:H:209:TYR:H	1.56	0.71
2:L:24:ARG:NH1	3:L:303:HOH:O	2.24	0.71
2:L:44:GLN:HA	2:L:48:LYS:HE2	1.74	0.70
2:L:211:VAL:O	3:L:301:HOH:O	2.09	0.70
2:L:56:LYS:NZ	3:L:306:HOH:O	2.25	0.69
1:H:138:PRO:HD3	1:H:224:LYS:HE2	1.76	0.65
1:H:179:HIS:NE2	3:H:303:HOH:O	2.27	0.65
2:L:149:THR:N	2:L:203:LYS:HE3	2.14	0.62
2:L:128:ARG:NH1	2:L:129:THR:O	2.34	0.61
2:L:45:ARG:H	2:L:48:LYS:HE2	1.65	0.61
1:H:112:LEU:HB2	2:L:109:SER:HA	1.86	0.58
2:L:21:ILE:HG23	3:L:307:HOH:O	2.03	0.57
2:L:186:GLN:HG2	2:L:191:SER:HA	1.86	0.57
1:H:1:GLU:OE1	1:H:3:GLN:NE2	2.39	0.56
1:H:196:VAL:HG21	2:L:155:LEU:HD22	1.89	0.54
2:L:187:ASP:O	2:L:191:SER:N	2.28	0.54
2:L:167:GLN:HB3	2:L:215:GLU:HB3	1.90	0.53
2:L:45:ARG:HD2	2:L:48:LYS:HD3	1.90	0.52
2:L:125:GLU:HG2	2:L:126:ILE:N	2.25	0.51
1:H:208:THR:HG22	1:H:209:TYR:N	2.24	0.51
3:H:301:HOH:O	2:L:68:GLU:OE1	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:140:PRO:HD3	2:L:152:VAL:HG22	1.95	0.49
2:L:158:ASN:OD1	2:L:192:THR:HG21	2.12	0.49
2:L:24:ARG:HH12	2:L:86:GLU:HB2	1.78	0.49
1:H:166:THR:OG1	1:H:214:ASN:HB3	2.12	0.49
2:L:148:GLY:H	2:L:203:LYS:HZ1	1.61	0.48
2:L:145:LEU:HA	2:L:203:LYS:HE2	1.94	0.48
1:H:30:PHE:CD2	1:H:85:SER:HA	2.48	0.48
2:L:45:ARG:H	2:L:48:LYS:HG2	1.78	0.47
1:H:4:LEU:HD22	1:H:23:CYS:SG	2.54	0.47
1:H:47:GLY:O	1:H:48:LYS:HD3	2.14	0.47
2:L:170:VAL:HA	3:L:301:HOH:O	2.15	0.47
2:L:144:GLN:HG2	2:L:149:THR:O	2.15	0.47
2:L:39:LEU:HG	2:L:40:ALA:N	2.29	0.47
2:L:43:GLN:HB2	2:L:53:LEU:HD11	1.96	0.46
1:H:134:PRO:HB3	1:H:160:TYR:HB3	1.98	0.46
2:L:53:LEU:HA	2:L:71:VAL:HG21	1.97	0.46
1:H:105:ALA:HB1	1:H:115:PHE:HB3	1.99	0.45
2:L:177:GLY:O	3:L:302:HOH:O	2.21	0.45
1:H:210:ILE:HA	1:H:224:LYS:C	2.36	0.45
2:L:148:GLY:N	2:L:203:LYS:HZ1	2.14	0.44
2:L:160:TYR:CG	2:L:161:PRO:HA	2.52	0.44
1:H:116:ASP:OD1	1:H:117:ILE:HD12	2.19	0.43
1:H:39:ILE:O	1:H:55:ILE:HG13	2.18	0.43
1:H:183:ALA:HA	1:H:193:LEU:HB3	2.00	0.43
2:L:171:ASP:OD2	2:L:209:HIS:HB3	2.19	0.43
2:L:183:VAL:HG12	2:L:184:THR:O	2.18	0.43
2:L:152:VAL:HB	2:L:199:LEU:HB3	2.01	0.43
2:L:6:GLN:HB3	3:L:307:HOH:O	2.19	0.43
2:L:79:SER:HB3	3:L:320:HOH:O	2.19	0.43
2:L:113:SER:HA	2:L:114:PRO:HD3	1.80	0.42
1:H:162:PRO:HD2	1:H:217:PRO:HB3	2.02	0.42
2:L:212:TYR:HA	3:L:301:HOH:O	2.20	0.42
1:H:158:LYS:NZ	1:H:186:GLN:OE1	2.53	0.41
2:L:24:ARG:HB2	2:L:24:ARG:CZ	2.48	0.41
1:H:66:ARG:CG	2:L:114:PRO:HG2	2.35	0.41
1:H:162:PRO:HD2	1:H:217:PRO:CB	2.51	0.41
2:L:148:GLY:H	2:L:203:LYS:NZ	2.20	0.40
2:L:37:SER:O	2:L:39:LEU:N	2.52	0.40
1:H:116:ASP:CG	1:H:117:ILE:HD12	2.41	0.40
2:L:128:ARG:HG2	2:L:129:THR:N	2.37	0.40
2:L:38:TRP:HB3	2:L:107:TYR:O	2.20	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	H	193/224 (86%)	186 (96%)	7 (4%)	0	100	100
2	L	201/216 (93%)	181 (90%)	17 (8%)	3 (2%)	12	16
All	All	394/440 (90%)	367 (93%)	24 (6%)	3 (1%)	22	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	38	TRP
2	L	177	GLY
2	L	110	TYR

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	H	169/191 (88%)	169 (100%)	0	100	100
2	L	181/190 (95%)	179 (99%)	2 (1%)	78	90
All	All	350/381 (92%)	348 (99%)	2 (1%)	89	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	203	LYS
2	L	222	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	170	ASN

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 carbohydrates 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, 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	H	199/224 (88%)	0.21	16 (8%) 13 12	14, 27, 72, 115	0
2	L	205/216 (94%)	0.64	27 (13%) 4 3	17, 39, 87, 105	0
All	All	404/440 (91%)	0.43	43 (10%) 7 6	14, 33, 78, 115	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	110	TYR	7.5
2	L	158	ASN	4.6
1	H	138	PRO	4.5
1	H	152	ALA	4.2
1	H	209	TYR	4.1
2	L	212	TYR	3.9
1	H	150	THR	3.7
2	L	109	SER	3.6
2	L	211	VAL	3.3
2	L	204	ALA	3.2
2	L	1	ASP	3.2
1	H	208	THR	3.1
2	L	205	ASP	3.1
2	L	148	GLY	3.0
2	L	206	TYR	3.0
2	L	114	PRO	2.9
1	H	173	ALA	2.9
2	L	167	GLN	2.8
1	H	151	ALA	2.8
2	L	207	GLU	2.8
2	L	145	LEU	2.8
2	L	225	VAL	2.7
2	L	150	ALA	2.7
1	H	174	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	151	SER	2.7
1	H	153	LEU	2.6
2	L	201	LEU	2.6
2	L	217	THR	2.6
1	H	139	LEU	2.5
1	H	176	SER	2.5
1	H	140	ALA	2.5
1	H	109	TYR	2.3
2	L	188	SER	2.3
2	L	157	ASN	2.3
2	L	141	SER	2.3
2	L	210	LYS	2.2
1	H	137	PHE	2.2
2	L	203	LYS	2.2
1	H	177	GLY	2.1
2	L	113	SER	2.1
2	L	189	LYS	2.1
1	H	136	VAL	2.0
2	L	152	VAL	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 [i](#)

There are no carbohydrates 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.