



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:23 am BST

PDB ID : 5OQI
Title : Crystal Structure of a disulfide trapped single chain trimer composed of the MHC I heavy chain H-2Kb Y84C E63A mutant, beta-2microglobulin, and ovalbumin-derived peptide
Authors : Mikolajek, H.; Werner, J.M.; Beton, M.E.
Deposited on : 2017-08-11
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

<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
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

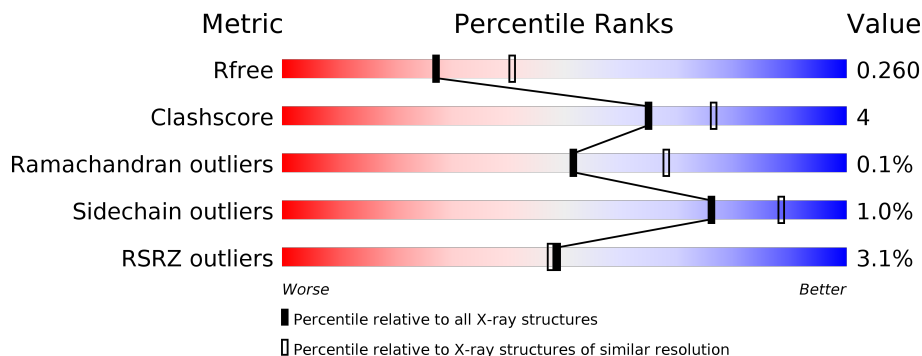
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 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	431	
1	B	431	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6661 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 Beta-2-microglobulin,H-2 class I histocompatibility antigen, K-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3146	1991	548	589	18	0	0	0
1	B	388	3146	1991	548	589	18	0	0	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P01887
A	2	ILE	-	expression tag	UNP P01887
A	3	ILE	-	expression tag	UNP P01887
A	4	ASN	-	expression tag	UNP P01887
A	5	PHE	-	expression tag	UNP P01887
A	6	GLU	-	expression tag	UNP P01887
A	7	LYS	-	expression tag	UNP P01887
A	8	LEU	-	expression tag	UNP P01887
A	9	GLY	-	expression tag	UNP P01887
A	10	CYS	-	expression tag	UNP P01887
A	11	GLY	-	expression tag	UNP P01887
A	12	ALA	-	expression tag	UNP P01887
A	13	SER	-	expression tag	UNP P01887
A	?	GLY	-	expression tag	UNP P01887
A	?	GLY	-	expression tag	UNP P01887
A	?	GLY	-	expression tag	UNP P01887
A	?	GLY	-	expression tag	UNP P01887
A	?	SER	-	expression tag	UNP P01887
A	?	GLY	-	expression tag	UNP P01887
A	?	GLY	-	expression tag	UNP P01887
A	?	GLY	-	expression tag	UNP P01887
A	?	GLY	-	expression tag	UNP P01887
A	?	GLY	-	expression tag	UNP P01887
A	?	GLY	-	expression tag	UNP P01887
A	?	SER	-	expression tag	UNP P01887
A	?	GLY	-	linker	UNP P01887

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	GLY	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	SER	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	SER	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	SER	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	GLY	-	linker	UNP P01887
A	?	SER	-	linker	UNP P01887
A	205	ALA	GLU	engineered mutation	UNP P01901
A	226	CYS	TYR	engineered mutation	UNP P01901
A	426	HIS	-	expression tag	UNP P01901
A	427	HIS	-	expression tag	UNP P01901
A	428	HIS	-	expression tag	UNP P01901
A	429	HIS	-	expression tag	UNP P01901
A	430	HIS	-	expression tag	UNP P01901
A	431	HIS	-	expression tag	UNP P01901
B	1	SER	-	expression tag	UNP P01887
B	2	ILE	-	expression tag	UNP P01887
B	3	ILE	-	expression tag	UNP P01887
B	4	ASN	-	expression tag	UNP P01887
B	5	PHE	-	expression tag	UNP P01887
B	6	GLU	-	expression tag	UNP P01887
B	7	LYS	-	expression tag	UNP P01887
B	8	LEU	-	expression tag	UNP P01887
B	9	GLY	-	expression tag	UNP P01887
B	10	CYS	-	expression tag	UNP P01887
B	11	GLY	-	expression tag	UNP P01887
B	12	ALA	-	expression tag	UNP P01887
B	13	SER	-	expression tag	UNP P01887
B	?	GLY	-	expression tag	UNP P01887
B	?	GLY	-	expression tag	UNP P01887

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	GLY	-	expression tag	UNP P01887
B	?	GLY	-	expression tag	UNP P01887
B	?	SER	-	expression tag	UNP P01887
B	?	GLY	-	expression tag	UNP P01887
B	?	GLY	-	expression tag	UNP P01887
B	?	GLY	-	expression tag	UNP P01887
B	?	GLY	-	expression tag	UNP P01887
B	?	SER	-	expression tag	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	SER	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	SER	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	SER	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	GLY	-	linker	UNP P01887
B	?	SER	-	linker	UNP P01887
B	205	ALA	GLU	engineered mutation	UNP P01901
B	226	CYS	TYR	engineered mutation	UNP P01901
B	426	HIS	-	expression tag	UNP P01901
B	427	HIS	-	expression tag	UNP P01901
B	428	HIS	-	expression tag	UNP P01901
B	429	HIS	-	expression tag	UNP P01901
B	430	HIS	-	expression tag	UNP P01901
B	431	HIS	-	expression tag	UNP P01901

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	204	Total O 204 204	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	165	Total 165	O 165	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.13Å 90.19Å 89.45Å 90.00° 111.22° 90.00°	Depositor
Resolution (Å)	42.52 – 2.40 42.52 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (42.52-2.40) 97.7 (42.52-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.201 , 0.260 0.201 , 0.260	Depositor DCC
R_{free} test set	1902 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtrriage
Anisotropy	0.740	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6661	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4935e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/3233	0.45	0/4387
1	B	0.24	0/3233	0.44	0/4387
All	All	0.24	0/6466	0.44	0/8774

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	A	3146	0	3015	25	0
1	B	3146	0	3015	25	0
2	A	204	0	0	5	0
2	B	165	0	0	3	0
All	All	6661	0	6030	50	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 (50) 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:224:LEU:HD21	1:B:231:LYS:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:NH1	1:A:161:GLU:O	2.28	0.66
1:A:339:ASP:N	1:A:339:ASP:OD1	2.25	0.66
1:B:214:GLN:NE2	1:B:217:ARG:HH21	1.97	0.63
1:B:214:GLN:HE22	1:B:217:ARG:HH21	1.47	0.62
1:A:204:ARG:NH1	2:A:501:HOH:O	2.27	0.62
1:A:161:GLU:OE1	1:A:217:ARG:NH1	2.35	0.59
1:A:286:LYS:NZ	2:A:504:HOH:O	2.36	0.58
1:B:3:ILE:HD13	1:B:298:LEU:HD23	1.87	0.57
1:B:10:CYS:SG	1:B:222:THR:HG22	2.46	0.55
1:B:71:LYS:HZ1	1:B:92:GLU:H	1.55	0.54
1:B:28:PRO:HB3	1:B:53:PHE:HB3	1.89	0.53
1:A:187:TYR:HE1	1:A:209:ALA:HB2	1.74	0.53
1:B:254:GLY:HA3	1:B:302:LEU:HD13	1.91	0.52
1:A:304:GLY:O	1:A:308:GLU:HG3	2.10	0.52
1:B:186:ARG:NH1	2:B:509:HOH:O	2.43	0.52
1:B:63:LEU:HD23	1:B:68:LYS:HA	1.92	0.52
1:A:60:ILE:HG12	1:A:105:VAL:HG22	1.92	0.51
1:A:253:ARG:NH2	2:A:509:HOH:O	2.42	0.51
1:A:40:ASN:HD21	1:A:97:GLU:HG3	1.76	0.51
1:B:156:ARG:HB3	1:B:159:LEU:HB2	1.93	0.50
1:B:70:PRO:O	2:B:501:HOH:O	2.20	0.50
1:A:156:ARG:NH2	2:A:511:HOH:O	2.45	0.50
1:B:76:ASP:OD2	1:B:190:ARG:NH2	2.43	0.50
1:B:71:LYS:NZ	1:B:92:GLU:HG3	2.27	0.49
1:A:81:LYS:HE2	1:A:148:ARG:HH22	1.76	0.49
1:A:119:ASP:O	1:A:122:MET:N	2.41	0.48
1:B:317:GLY:O	1:B:321:LEU:HD22	2.13	0.48
1:B:187:TYR:HE1	1:B:209:ALA:HB2	1.78	0.48
1:B:11:GLY:HA3	1:B:284:ILE:HD13	1.95	0.48
1:B:3:ILE:CD1	1:B:298:LEU:HD23	2.43	0.47
1:A:155:SER:HB3	1:A:220:LEU:HD13	1.97	0.46
1:A:24:ILE:N	2:A:513:HOH:O	2.48	0.46
1:B:256:GLN:HG3	1:B:298:LEU:HD22	1.98	0.45
1:B:3:ILE:HD13	1:B:298:LEU:CD2	2.46	0.45
1:B:186:ARG:NH2	1:B:203:GLU:HA	2.32	0.44
1:A:71:LYS:HA	1:A:71:LYS:HD3	1.72	0.44
1:A:13:SER:OG	1:A:225:GLY:HA3	2.18	0.43
1:A:206:THR:HG22	1:A:210:LYS:HD2	1.99	0.43
1:B:83:TRP:CE2	1:B:259:ALA:HB2	2.54	0.43
1:A:154:VAL:HG22	1:A:236:THR:HG22	2.01	0.43
1:A:64:LYS:HB3	1:A:69:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:HG3	2:B:506:HOH:O	2.19	0.42
1:A:64:LYS:HE3	1:A:64:LYS:HB2	1.80	0.42
1:B:269:ASN:OD1	1:B:274:THR:HG23	2.19	0.42
1:B:280:MET:HA	1:B:283:LEU:HD12	2.01	0.41
1:A:40:ASN:OD1	1:A:120:ARG:NH2	2.53	0.41
1:A:64:LYS:HG3	1:A:64:LYS:O	2.20	0.41
1:A:63:LEU:HD23	1:A:68:LYS:HA	2.03	0.40
1:A:156:ARG:HB2	1:A:159:LEU:HD12	2.04	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	A	382/431 (89%)	370 (97%)	12 (3%)	0	100	100
1	B	382/431 (89%)	370 (97%)	11 (3%)	1 (0%)	41	55
All	All	764/862 (89%)	740 (97%)	23 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	PRO

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	336/355 (95%)	331 (98%)	5 (2%)	65	80
1	B	336/355 (95%)	334 (99%)	2 (1%)	86	94
All	All	672/710 (95%)	665 (99%)	7 (1%)	76	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LYS
1	A	93	PHE
1	A	156	ARG
1	A	165	MET
1	A	187	TYR
1	B	71	LYS
1	B	187	TYR

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

Mol	Chain	Res	Type
1	B	214	GLN

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	A	388/431 (90%)	0.00	18 (4%) 32 31	22, 37, 58, 75	0
1	B	388/431 (90%)	-0.05	6 (1%) 73 72	20, 36, 54, 78	0
All	All	776/862 (90%)	-0.02	24 (3%) 49 47	20, 37, 56, 78	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	SER	5.0
1	A	143	GLY	4.9
1	B	183	GLU	4.2
1	A	122	MET	4.1
1	A	319	ALA	3.1
1	A	183	GLU	3.1
1	A	317	GLY	3.0
1	B	143	GLY	3.0
1	A	231	LYS	2.8
1	A	320	THR	2.7
1	B	368	GLN	2.7
1	A	368	GLN	2.7
1	A	322	LEU	2.6
1	A	318	ASN	2.5
1	A	369	ASP	2.5
1	A	12	ALA	2.5
1	B	231	LYS	2.4
1	A	337	PRO	2.4
1	A	321	LEU	2.3
1	A	367	ILE	2.2
1	A	323	ARG	2.2
1	B	369	ASP	2.2
1	B	182	ALA	2.1
1	A	182	ALA	2.1

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.