



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:47 PM GMT

PDB ID : 2QRT
Title : Crystal Structure of a disulfide trapped single chain trimer composed of the MHC I heavy chain H-2Kb Y84C, beta-2microglobulin, and ovalbumin-derived peptide.
Authors : Mitaksov, V.E.; Fremont, D.H.
Deposited on : 2007-07-29
Resolution : 1.80 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

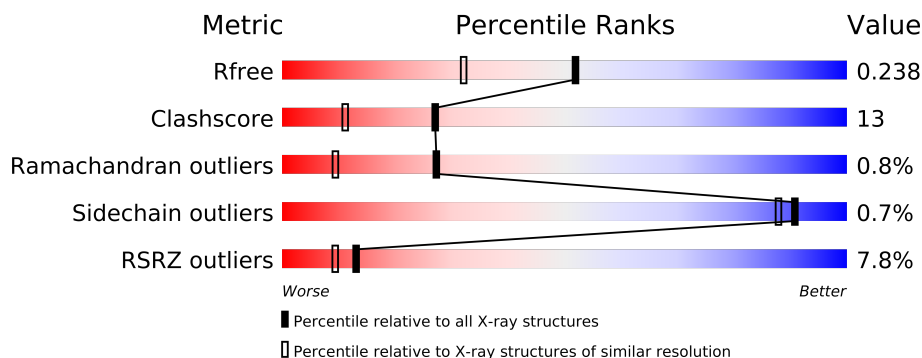
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.80 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}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	422	
1	B	422	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7143 atoms, of which 0 are hydrogen and 0 are deuterium.

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 H-2 class I histocompatibility antigen K-B alpha chain, Beta-2 microglobulin, ovalbumin-derived peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3194	2015	558	603	18			
1	B	398	Total	C	N	O	S	0	0	0
			3194	2015	558	603	18			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9P	GLY	-	linker	UNP P01901
A	10P	CYS	-	linker	UNP P01901
A	11P	GLY	-	linker	UNP P01901
A	12P	ALA	-	linker	UNP P01901
A	13P	SER	-	linker	UNP P01901
A	14P	GLY	-	linker	UNP P01901
A	15P	GLY	-	linker	UNP P01901
A	16P	GLY	-	linker	UNP P01901
A	17P	GLY	-	linker	UNP P01901
A	18P	SER	-	linker	UNP P01901
A	19P	GLY	-	linker	UNP P01901
A	20P	GLY	-	linker	UNP P01901
A	21P	GLY	-	linker	UNP P01901
A	22P	GLY	-	linker	UNP P01901
A	23P	SER	-	linker	UNP P01901
A	100B	GLY	-	linker	UNP P01901
A	101B	GLY	-	linker	UNP P01901
A	102B	GLY	-	linker	UNP P01901
A	103B	GLY	-	linker	UNP P01901
A	104B	SER	-	linker	UNP P01901
A	105B	GLY	-	linker	UNP P01901
A	106B	GLY	-	linker	UNP P01901
A	107B	GLY	-	linker	UNP P01901
A	108B	GLY	-	linker	UNP P01901

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Chain	Residue	Modelled	Actual	Comment	Reference
A	109B	SER	-	linker	UNP P01901
A	110B	GLY	-	linker	UNP P01901
A	111B	GLY	-	linker	UNP P01901
A	112B	GLY	-	linker	UNP P01901
A	113B	GLY	-	linker	UNP P01901
A	114B	SER	-	linker	UNP P01901
A	115B	GLY	-	linker	UNP P01901
A	116B	GLY	-	linker	UNP P01901
A	117B	GLY	-	linker	UNP P01901
A	118B	GLY	-	linker	UNP P01901
A	119B	SER	-	linker	UNP P01901
A	84H	CYS	TYR	engineered	UNP P01901
B	9P	GLY	-	linker	UNP P01901
B	10P	CYS	-	linker	UNP P01901
B	11P	GLY	-	linker	UNP P01901
B	12P	ALA	-	linker	UNP P01901
B	13P	SER	-	linker	UNP P01901
B	14P	GLY	-	linker	UNP P01901
B	15P	GLY	-	linker	UNP P01901
B	16P	GLY	-	linker	UNP P01901
B	17P	GLY	-	linker	UNP P01901
B	18P	SER	-	linker	UNP P01901
B	19P	GLY	-	linker	UNP P01901
B	20P	GLY	-	linker	UNP P01901
B	21P	GLY	-	linker	UNP P01901
B	22P	GLY	-	linker	UNP P01901
B	23P	SER	-	linker	UNP P01901
B	100B	GLY	-	linker	UNP P01901
B	101B	GLY	-	linker	UNP P01901
B	102B	GLY	-	linker	UNP P01901
B	103B	GLY	-	linker	UNP P01901
B	104B	SER	-	linker	UNP P01901
B	105B	GLY	-	linker	UNP P01901
B	106B	GLY	-	linker	UNP P01901
B	107B	GLY	-	linker	UNP P01901
B	108B	GLY	-	linker	UNP P01901
B	109B	SER	-	linker	UNP P01901
B	110B	GLY	-	linker	UNP P01901
B	111B	GLY	-	linker	UNP P01901
B	112B	GLY	-	linker	UNP P01901
B	113B	GLY	-	linker	UNP P01901
B	114B	SER	-	linker	UNP P01901

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Chain	Residue	Modelled	Actual	Comment	Reference
B	115B	GLY	-	linker	UNP P01901
B	116B	GLY	-	linker	UNP P01901
B	117B	GLY	-	linker	UNP P01901
B	118B	GLY	-	linker	UNP P01901
B	119B	SER	-	linker	UNP P01901
B	84H	CYS	TYR	engineered	UNP P01901

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	368	Total O 368 368	0	0
2	B	387	Total O 387 387	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	66.60Å 89.10Å 88.60Å 90.00° 110.90° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 19.93 – 1.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.80) 99.7 (19.93-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.76Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.239 0.207 , 0.238	Depositor DCC
R_{free} test set	4501 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.5	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 96862 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7143	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.61 % 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 2.3021e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	A	0.45	0/3282	0.73	3/4451 (0.1%)
1	B	0.44	0/3282	0.70	1/4451 (0.0%)
All	All	0.45	0/6564	0.71	4/8902 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272(H)	LEU	CA-CB-CG	7.52	132.60	115.30
1	A	19(P)	GLY	N-CA-C	-6.81	96.08	113.10
1	A	230(H)	LEU	CA-CB-CG	5.89	128.84	115.30
1	A	1(B)	ILE	N-CA-C	-5.20	96.97	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3194	0	3054	87	0
1	B	3194	0	3054	76	0
2	A	368	0	0	18	0
2	B	387	0	0	29	0
All	All	7143	0	6108	162	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

The worst 5 of 162 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99(B):MET:HB2	1:A:192(H):HIS:HE1	1.14	1.09
1:A:23(P):SER:HB3	1:A:119(H):ASP:HB3	1.37	1.03
1:A:77(B):THR:HB	2:A:648:HOH:O	1.63	0.98
1:A:99(B):MET:HB2	1:A:192(H):HIS:CE1	1.99	0.97
1:B:15(P):GLY:O	1:B:84(H):CYS:HA	1.70	0.92

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	394/422 (93%)	377 (96%)	14 (4%)	3 (1%)	27	9
1	B	394/422 (93%)	371 (94%)	20 (5%)	3 (1%)	27	9
All	All	788/844 (93%)	748 (95%)	34 (4%)	6 (1%)	27	9

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176(H)	ASN
1	B	17(H)	LEU
1	A	98(B)	ASP
1	B	197(H)	ASP
1	A	21(P)	GLY

5.3.2 Protein sidechains ⓘ

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	339/347 (98%)	337 (99%)	2 (1%)	92	90
1	B	339/347 (98%)	336 (99%)	3 (1%)	87	83
All	All	678/694 (98%)	673 (99%)	5 (1%)	91	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70(B)	PHE
1	A	45(H)	TYR
1	B	70(B)	PHE
1	B	45(H)	TYR
1	B	230(H)	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	8(B)	GLN
1	B	42(H)	ASN
1	B	226(H)	GLN
1	B	6(B)	GLN
1	B	174(H)	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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, 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	398/422 (94%)	0.24	27 (6%) 17 12	20, 31, 61, 94	0
1	B	398/422 (94%)	0.25	35 (8%) 10 7	19, 32, 62, 93	0
All	All	796/844 (94%)	0.24	62 (7%) 13 9	19, 32, 62, 94	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16(P)	GLY	14.5
1	A	17(P)	GLY	14.5
1	A	23(P)	SER	14.2
1	A	21(P)	GLY	14.1
1	A	19(P)	GLY	13.9

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 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.