wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 01:27 pm BST

PDB ID	:	4ZDH
Title	:	Crystal structure of JKA6 TCR
Authors	:	Singh, N.K.; Hossain, M.; Baker, B.M.
Deposited on	:	2015-04-17
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

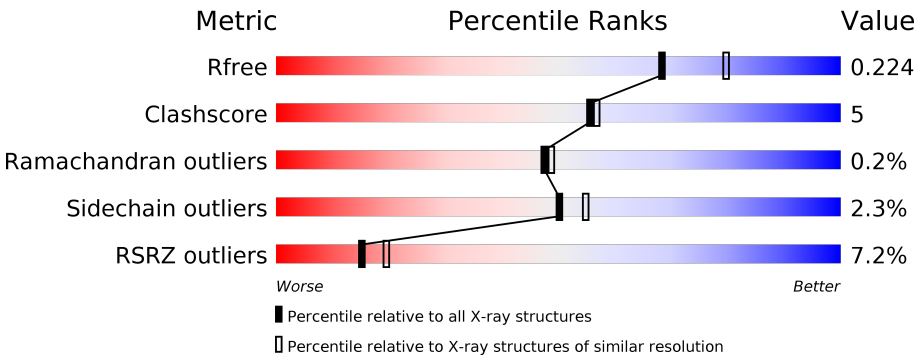
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	A	201	10% 88% 10% •
2	B	241	5% 85% 14% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3641 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 Alpha chain of A6 T-cell receptor,T-cell receptor alpha chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	1556	968	255	325	8	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	SER	-	conflict	PDB ?
A	80	ALA	-	conflict	PDB ?
A	93	THR	-	conflict	PDB ?
A	94	THR	-	linker	PDB ?
A	95	ASP	-	linker	PDB ?
A	96	SER	-	linker	PDB ?
A	97	TRP	-	linker	PDB ?
A	98	GLY	-	linker	PDB ?
A	99	LYS	-	linker	PDB ?
A	100	LEU	-	linker	PDB ?
A	101	GLN	-	linker	PDB ?
A	102	PHE	-	linker	PDB ?
A	103	GLY	-	linker	PDB ?
A	104	ALA	-	linker	PDB ?
A	105	GLY	-	linker	PDB ?
A	106	THR	-	linker	PDB ?
A	107	GLN	-	linker	PDB ?
A	108	VAL	-	linker	PDB ?
A	109	VAL	-	linker	PDB ?
A	110	VAL	-	linker	PDB ?
A	111	THR	-	linker	PDB ?
A	112	PRO	-	linker	PDB ?
A	113	ASP	-	linker	PDB ?
A	160	CYS	THR	conflict	UNP P01848

- Molecule 2 is a protein called Beta chain of JKF6 T-cell receptor,Protein TRBV28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	241	1935	1228	330	368	9	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	79	ALA	-	conflict	PDB ?
B	84	ASP	-	conflict	PDB ?
B	95	PHE	-	conflict	PDB ?
B	96	LEU	-	linker	PDB ?
B	97	GLY	-	linker	PDB ?
B	98	THR	-	linker	PDB ?
B	99	GLY	-	linker	PDB ?
B	100	VAL	-	linker	PDB ?
B	101	GLU	-	linker	PDB ?
B	102	GLN	-	linker	PDB ?
B	103	TYR	-	linker	PDB ?
B	104	PHE	-	linker	PDB ?
B	105	GLY	-	linker	PDB ?
B	106	PRO	-	linker	PDB ?
B	126	LEU	VAL	conflict	UNP A0A087WZV8
B	150	TYR	PHE	conflict	UNP A0A087WZV8
B	170	CYS	SER	conflict	UNP A0A087WZV8
B	188	ALA	CYS	conflict	UNP A0A087WZV8
B	202	ASP	ASN	conflict	UNP A0A087WZV8
B	219	ALA	ASN	conflict	UNP A0A087WZV8
B	225	ALA	ASP	conflict	UNP A0A087WZV8

- Molecule 3 is water.

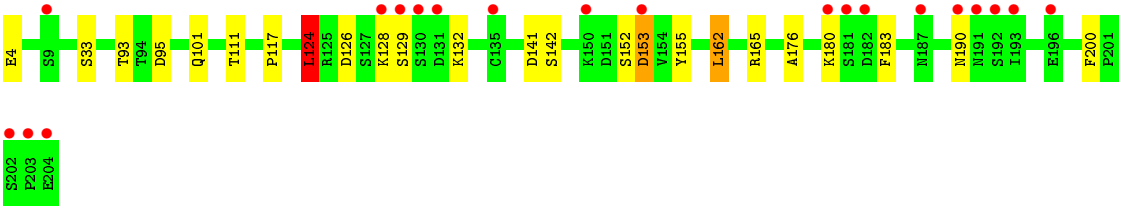
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	60	60	60	0	0
			Total	O		
3	B	90	90	90	0	0

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.

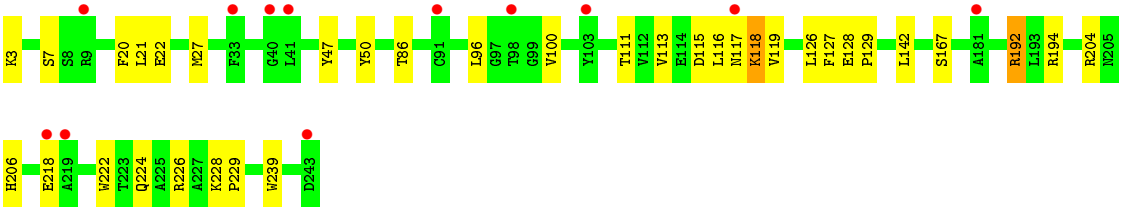
- Molecule 1: Alpha chain of A6 T-cell receptor,T-cell receptor alpha chain C region

Chain A:



- Molecule 2: Beta chain of JKF6 T-cell receptor,Protein TRBV28

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.70Å 60.09Å 82.46Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	19.49 – 2.10 19.49 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.1 (19.49-2.10) 95.1 (19.49-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.09Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.190 , 0.224 0.190 , 0.224	Depositor DCC
R_{free} test set	1263 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3641	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% 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 (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	0.38	0/1590	0.59	2/2160 (0.1%)
2	B	0.42	0/1985	0.57	0/2692
All	All	0.40	0/3575	0.58	2/4852 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162	LEU	CA-CB-CG	5.78	128.60	115.30
1	A	124	LEU	CA-CB-CG	5.31	127.50	115.30

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	1556	0	1455	18	0
2	B	1935	0	1863	23	0
3	A	60	0	0	0	0
3	B	90	0	0	1	0
All	All	3641	0	3318	35	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 5.

The worst 5 of 35 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:A:126:ASP:HB3	1:A:129:SER:O	2.02	0.60
1:A:180:LYS:HB2	1:A:183:PHE:HB2	1.90	0.54
1:A:165:ARG:HG3	2:B:167:SER:OG	2.09	0.53
1:A:33:SER:HB2	1:A:93:THR:HG23	1.90	0.53
1:A:132:LYS:HG3	2:B:127:PHE:CE2	2.45	0.53

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	199/201 (99%)	195 (98%)	3 (2%)	1 (0%)	29	26
2	B	239/241 (99%)	234 (98%)	5 (2%)	0	100	100
All	All	438/442 (99%)	429 (98%)	8 (2%)	1 (0%)	47	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ASN

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	178/178 (100%)	174 (98%)	4 (2%)	52	57
2	B	211/211 (100%)	206 (98%)	5 (2%)	49	53
All	All	389/389 (100%)	380 (98%)	9 (2%)	50	55

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	47	TYR
2	B	192	ARG
2	B	100	VAL
1	A	153	ASP
2	B	96	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (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, 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	201/201 (100%)	0.45	20 (9%)	7	9	24, 37, 90, 121	1 (0%)
2	B	241/241 (100%)	0.11	12 (4%)	28	34	22, 33, 57, 94	0
All	All	442/442 (100%)	0.26	32 (7%)	15	19	22, 35, 73, 121	1 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	SER	8.1
1	A	204	GLU	6.3
1	A	131	ASP	6.3
1	A	182	ASP	5.7
1	A	181	SER	5.6

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.