



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:57 PM GMT

PDB ID : 4MXQ
Title : 42F3 TCR pCPC5/H-2Ld Complex
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Deposited on : 2013-09-26
Resolution : 2.60 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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20026982

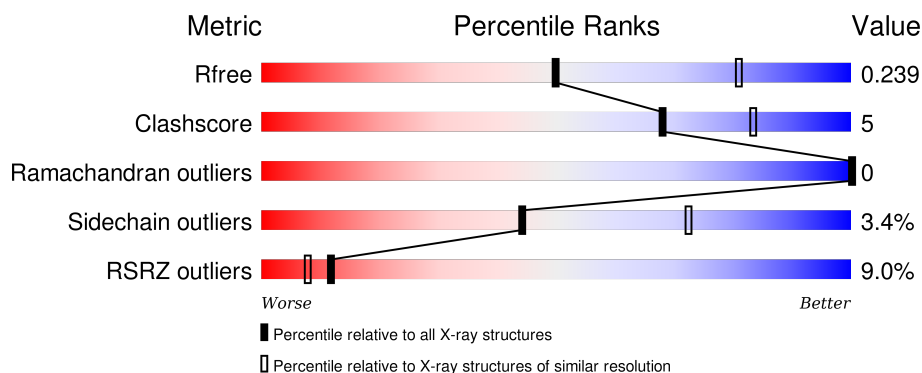
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	C	212	<div> <div>20%</div> <div>76%</div> <div>16%</div> <div>• 6%</div> </div>
2	D	243	<div> <div>4%</div> <div>86%</div> <div>12%</div> <div>•</div> </div>
3	A	180	<div> <div>3%</div> <div>86%</div> <div>10%</div> <div>• •</div> </div>
4	B	9	<div> <div>56%</div> <div>44%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4958 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 42F3 alpha VmVh chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	199	Total	C	N	O	S	0	0	0
			1534	968	255	303	8			

- Molecule 2 is a protein called 42F3 beta VmVh chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	239	Total	C	N	O	S	0	0	0
			1891	1192	329	364	6			

- Molecule 3 is a protein called H-2 class I histocompatibility antigen, L-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	174	Total	C	N	O	S	0	0	0
			1444	909	253	275	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	UNP P01897
A	8	TYR	PHE	ENGINEERED MUTATION	UNP P01897
A	12	THR	VAL	ENGINEERED MUTATION	UNP P01897
A	15	ARG	PRO	ENGINEERED MUTATION	UNP P01897
A	23	THR	ILE	ENGINEERED MUTATION	UNP P01897
A	30	ASP	ASN	ENGINEERED MUTATION	UNP P01897
A	49	VAL	ALA	ENGINEERED MUTATION	UNP P01897
A	131	ARG	LYS	ENGINEERED MUTATION	UNP P01897

- Molecule 4 is a protein called pCPC5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	9	Total	C	N	O	0	0	0
			68	43	12	13			

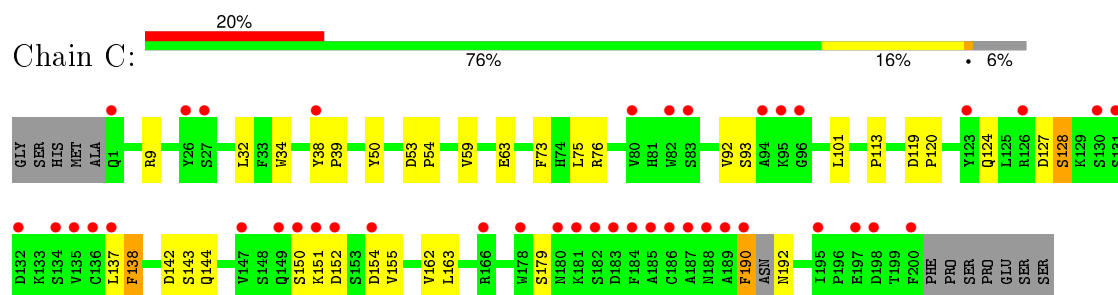
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	5	Total 5	O 5	0	0
5	D	10	Total 10	O 10	0	0
5	A	6	Total 6	O 6	0	0

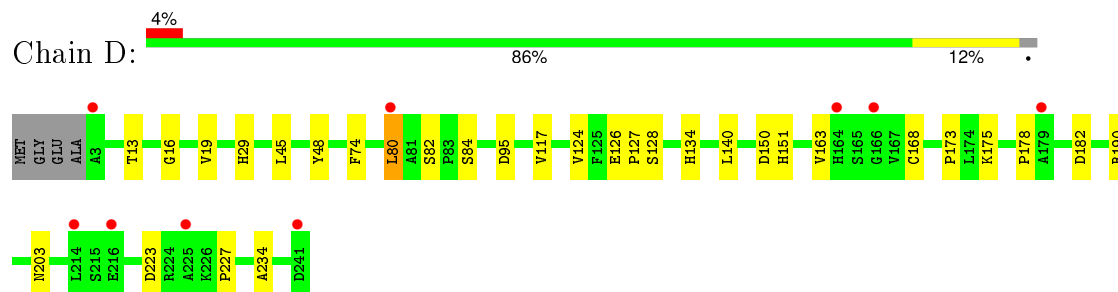
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

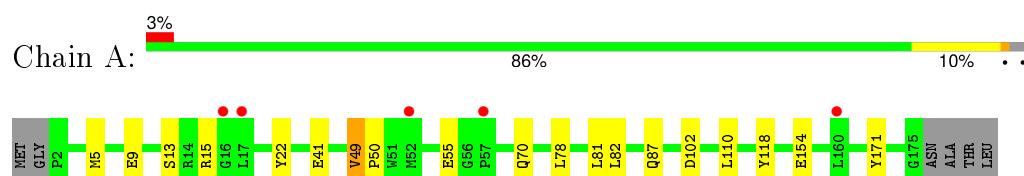
- Molecule 1: 42F3 alpha VmVh chimera



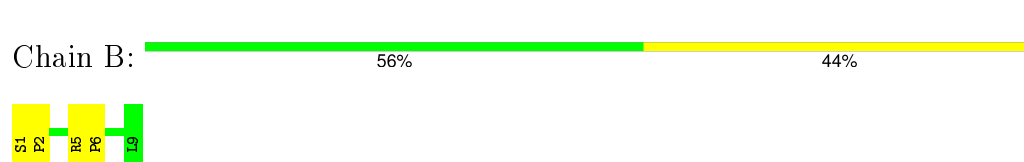
- Molecule 2: 42F3 beta VmVh chimera



- Molecule 3: H-2 class I histocompatibility antigen, L-D alpha chain



- Molecule 4: pCPC5



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.72Å 102.72Å 322.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.33 – 2.60 59.78 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.4 (43.33-2.60) 95.0 (59.78-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.211 , 0.240 0.207 , 0.239	Depositor DCC
R_{free} test set	1546 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30776 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4958	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	C	0.25	0/1570	0.46	0/2127
2	D	0.23	0/1943	0.44	0/2650
3	A	0.26	0/1486	0.43	0/2015
4	B	0.18	0/70	0.43	0/95
All	All	0.25	0/5069	0.44	0/6887

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	C	1534	0	1451	20	0
2	D	1891	0	1787	16	0
3	A	1444	0	1320	11	0
4	B	68	0	72	3	0
5	A	6	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	2	0
All	All	4958	0	4630	45	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.

All (45) 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)
2:D:203:ASN:OD1	5:D:308:HOH:O	2.15	0.60
1:C:63:GLU:OE2	1:C:76:ARG:NH2	2.31	0.59
3:A:5:MET:HE3	3:A:171:TYR:HE2	1.67	0.59
2:D:16:GLY:HA2	2:D:80:LEU:HD13	1.83	0.59
1:C:50:TYR:HB2	3:A:154:GLU:HG2	1.84	0.59
3:A:5:MET:HE3	3:A:171:TYR:CE2	2.40	0.57
3:A:41:GLU:OE1	3:A:41:GLU:N	2.37	0.57
2:D:127:PRO:HD3	2:D:140:LEU:HG	1.86	0.57
3:A:13:SER:HB3	3:A:78:LEU:HD13	1.87	0.56
1:C:138:PHE:HB2	1:C:190:PHE:CZ	2.40	0.56
1:C:190:PHE:O	1:C:192:ASN:N	2.39	0.55
1:C:150:SER:OG	1:C:151:LYS:N	2.39	0.55
1:C:127:ASP:OD1	1:C:128:SER:N	2.42	0.53
2:D:82:SER:HG	2:D:84:SER:HG	1.57	0.52
2:D:124:VAL:HG23	2:D:234:ALA:HB3	1.93	0.51
1:C:152:ASP:HB3	1:C:155:VAL:HG22	1.91	0.51
1:C:32:LEU:HD13	1:C:73:PHE:HB2	1.94	0.50
2:D:29:HIS:CD2	2:D:95:ASP:HB3	2.48	0.49
1:C:155:VAL:HA	1:C:179:SER:HB2	1.96	0.48
1:C:113:PRO:HG3	1:C:162:VAL:HG11	1.95	0.48
2:D:150:ASP:OD1	2:D:173:PRO:HG2	2.13	0.48
3:A:70:GLN:HE22	4:B:5:ARG:HA	1.79	0.47
1:C:113:PRO:O	1:C:143:SER:OG	2.22	0.47
1:C:34:TRP:CE2	1:C:75:LEU:HB2	2.49	0.47
1:C:144:GLN:OE1	1:C:144:GLN:N	2.48	0.47
2:D:117:VAL:HG12	2:D:227:PRO:HB2	1.98	0.46
2:D:175:LYS:HE2	2:D:178:PRO:HA	1.97	0.46
1:C:128:SER:OG	2:D:126:GLU:OE2	2.23	0.46
1:C:124:GLN:O	2:D:128:SER:HB2	2.16	0.46
3:A:49:VAL:HG22	3:A:50:PRO:HD2	1.97	0.46
1:C:163:LEU:HB3	2:D:168:CYS:HB2	1.98	0.45
1:C:53:ASP:HA	1:C:54:PRO:HD3	1.84	0.44
1:C:38:TYR:HB3	1:C:39:PRO:HD2	1.99	0.44
2:D:163:VAL:O	5:D:304:HOH:O	2.21	0.43
4:B:1:SER:HA	4:B:2:PRO:HD3	1.94	0.42
3:A:102:ASP:O	3:A:110:LEU:N	2.51	0.42
2:D:13:THR:HG21	2:D:19:VAL:HG22	2.01	0.42
1:C:93:SER:HB3	1:C:101:LEU:HD23	2.02	0.42
3:A:82:LEU:HD23	3:A:87:GLN:HB2	2.02	0.42
3:A:9:GLU:OE1	3:A:22:TYR:OH	2.28	0.41
2:D:182:ASP:N	2:D:182:ASP:OD1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ASP:HA	1:C:120:PRO:HD2	1.88	0.41
4:B:5:ARG:HA	4:B:6:PRO:HD3	1.97	0.40
3:A:81:LEU:HD13	3:A:118:TYR:CD1	2.56	0.40
2:D:45:LEU:HD21	2:D:48:TYR:CD2	2.56	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	C	195/212 (92%)	190 (97%)	5 (3%)	0	100	100
2	D	237/243 (98%)	229 (97%)	8 (3%)	0	100	100
3	A	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
4	B	7/9 (78%)	7 (100%)	0	0	100	100
All	All	611/644 (95%)	592 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	C	170/186 (91%)	161 (95%)	9 (5%)	28	53
2	D	205/208 (99%)	199 (97%)	6 (3%)	50	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	143/148 (97%)	140 (98%)	3 (2%)	61	85
4	B	8/8 (100%)	8 (100%)	0	100	100
All	All	526/550 (96%)	508 (97%)	18 (3%)	44	72

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	9	ARG
1	C	59	VAL
1	C	92	VAL
1	C	128	SER
1	C	137	LEU
1	C	138	PHE
1	C	142	ASP
1	C	154	ASP
1	C	190	PHE
2	D	74	PHE
2	D	80	LEU
2	D	134	HIS
2	D	151	HIS
2	D	190	ARG
2	D	223	ASP
3	A	15	ARG
3	A	49	VAL
3	A	55	GLU

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

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 [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	C	199/212 (93%)	1.18	42 (21%) 1 0	58, 91, 152, 164	0
2	D	239/243 (98%)	0.59	9 (3%) 44 36	53, 78, 121, 147	0
3	A	174/180 (96%)	0.57	5 (2%) 55 48	56, 81, 124, 142	0
4	B	9/9 (100%)	0.36	0 100 100	57, 64, 75, 87	0
All	All	621/644 (96%)	0.77	56 (9%) 12 8	53, 82, 134, 164	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	184	PHE	6.3
1	C	182	SER	5.8
1	C	186	CYS	5.2
1	C	189	ALA	4.5
1	C	190	PHE	4.4
2	D	241	ASP	4.3
1	C	183	ASP	4.2
1	C	185	ALA	4.1
1	C	131	SER	4.0
1	C	187	ALA	4.0
1	C	126	ARG	3.7
1	C	188	ASN	3.5
3	A	16	GLY	3.5
3	A	17	LEU	3.4
1	C	152	ASP	3.3
1	C	132	ASP	3.2
1	C	181	LYS	3.2
1	C	96	GLY	3.1
1	C	26	TYR	3.0
2	D	225	ALA	2.9
1	C	135	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	27	SER	2.9
1	C	198	ASP	2.8
2	D	3	ALA	2.8
1	C	1	GLN	2.8
1	C	149	GLN	2.8
1	C	134	SER	2.8
1	C	197	GLU	2.7
1	C	150	SER	2.7
1	C	200	PHE	2.6
1	C	195	ILE	2.6
1	C	147	VAL	2.6
1	C	178	TRP	2.6
1	C	83	SER	2.5
2	D	166	GLY	2.5
1	C	154	ASP	2.4
1	C	130	SER	2.4
3	A	52	MET	2.3
3	A	160	LEU	2.3
2	D	214	LEU	2.3
1	C	95	LYS	2.3
1	C	136	CYS	2.2
1	C	180	ASN	2.2
2	D	164	HIS	2.1
1	C	80	VAL	2.1
2	D	179	ALA	2.1
1	C	38	TYR	2.1
1	C	166	ARG	2.1
1	C	137	LEU	2.1
3	A	57	PRO	2.1
1	C	123	TYR	2.1
1	C	82	TRP	2.1
1	C	151	LYS	2.1
1	C	94	ALA	2.0
2	D	216	GLU	2.0
2	D	80	LEU	2.0

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 [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.