



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 20, 2018 – 04:12 PM EDT

PDB ID : 4N0C
Title : 42F3 TCR pCPE3/H-2Ld complex
Authors : Birnbaum, M.E.; Adams, J.J.; Garcia, K.C.
Deposited on : 2013-10-01
Resolution : 2.90 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 ⓘ 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 : rb-20031172
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

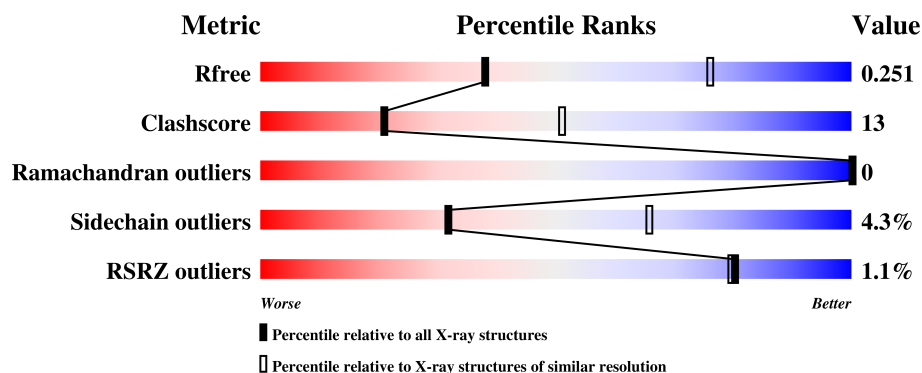
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

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	A	180	<div> <div>68%</div> <div>28%</div> <div>.</div> </div>
1	E	180	<div> <div>73%</div> <div>22%</div> <div>..</div> </div>
2	B	9	<div> <div>11%</div> <div>56%</div> <div>44%</div> </div>
2	F	9	<div> <div>67%</div> <div>33%</div> </div>
3	C	212	<div> <div>2%</div> <div>60%</div> <div>29%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	212	<div><div>%</div><div><div></div><div>63%</div><div>27%</div><div>7%</div></div><div></div></div>
4	D	243	<div><div>%</div><div><div></div><div>70%</div><div>27%</div><div></div></div><div></div></div>
4	H	243	<div><div></div><div><div></div><div>70%</div><div>27%</div><div></div></div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9790 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 H-2 class I histocompatibility antigen, L-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1437	904	253	274	6			
1	E	174	Total	C	N	O	S	0	0	0
			1444	910	254	273	7			

There are 16 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
E	0	MET	-	INITIATING METHIONINE	UNP P01897
E	8	TYR	PHE	ENGINEERED MUTATION	UNP P01897
E	12	THR	VAL	ENGINEERED MUTATION	UNP P01897
E	15	ARG	PRO	ENGINEERED MUTATION	UNP P01897
E	23	THR	ILE	ENGINEERED MUTATION	UNP P01897
E	30	ASP	ASN	ENGINEERED MUTATION	UNP P01897
E	49	VAL	ALA	ENGINEERED MUTATION	UNP P01897
E	131	ARG	LYS	ENGINEERED MUTATION	UNP P01897

- Molecule 2 is a protein called pCPE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	S	0	0	0
			73	47	13	12	1			
2	F	9	Total	C	N	O	S	0	0	0
			73	47	13	12	1			

- Molecule 3 is a protein called 42F3 VmCh alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	195	Total	C	N	O	S	0	0	0
			1488	930	252	298	8			
3	G	197	Total	C	N	O	S	0	0	0
			1505	946	248	303	8			

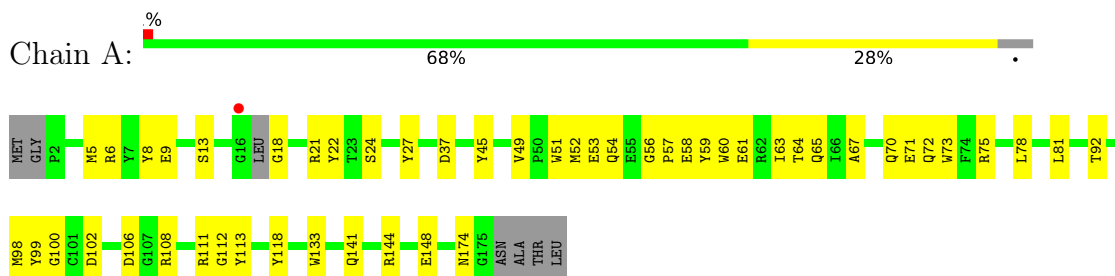
- Molecule 4 is a protein called 42F3 VmCh beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1891	1192	329	364	6			
4	H	239	Total	C	N	O	S	0	0	0
			1879	1183	325	365	6			

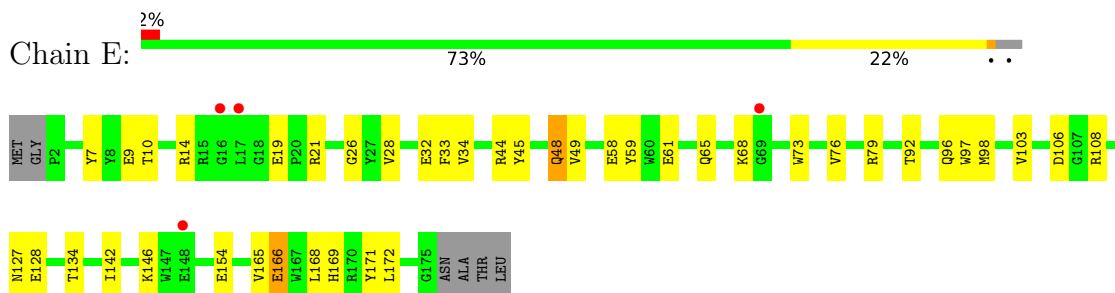
3 Residue-property plots [i](#)

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



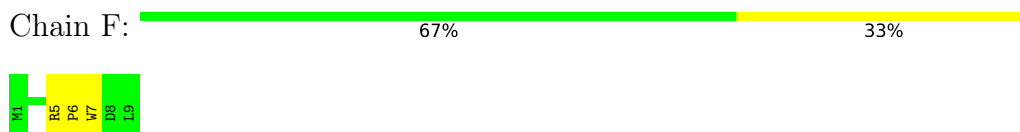
- Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain



- Molecule 2: pCPE3

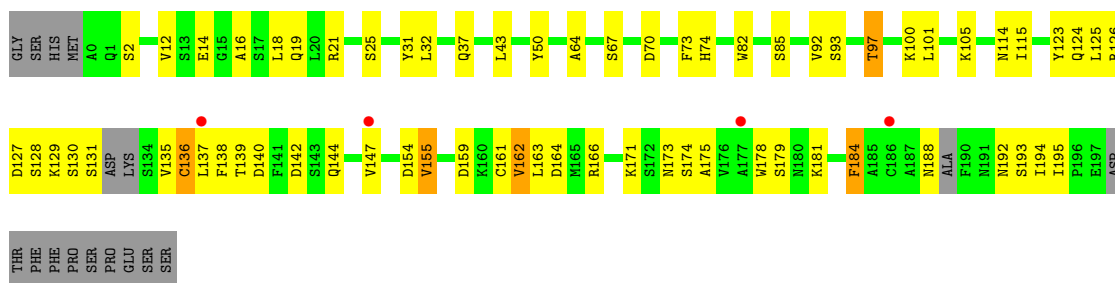


- Molecule 2: pCPE3

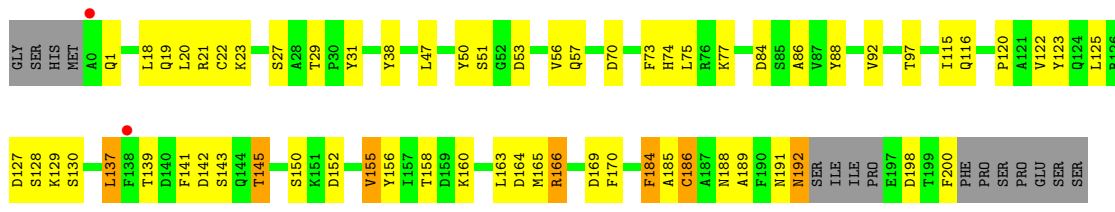


- Molecule 3: 42F3 VmCh alpha

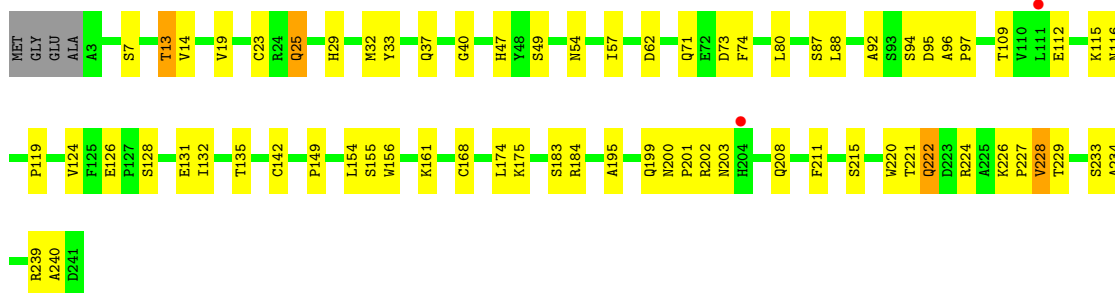




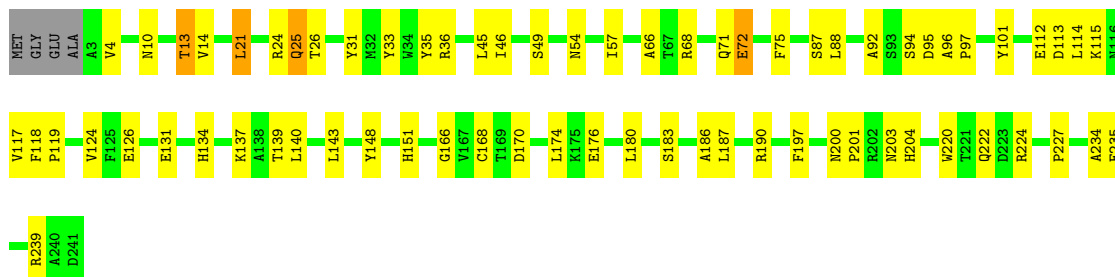
• Molecule 3: 42F3 VmCh alpha



• Molecule 4: 42F3 VmCh beta



• Molecule 4: 42F3 VmCh beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.45Å 102.45Å 325.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.99 – 2.90 59.99 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.4 (59.99-2.90) 99.2 (59.99-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.192 , 0.247 0.194 , 0.251	Depositor DCC
R_{free} test set	2823 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	71.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.439 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9790	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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 [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	0.32	0/1478	0.47	0/2002
1	E	0.29	0/1486	0.45	0/2014
2	B	0.26	0/76	0.51	0/102
2	F	0.24	0/76	0.37	0/102
3	C	0.35	0/1519	0.55	0/2057
3	G	0.33	0/1539	0.51	0/2086
4	D	0.34	0/1943	0.50	0/2650
4	H	0.34	0/1930	0.50	0/2634
All	All	0.33	0/10047	0.50	0/13647

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	1437	0	1312	41	0
1	E	1444	0	1327	29	0
2	B	73	0	71	4	0
2	F	73	0	71	3	0
3	C	1488	0	1408	45	0
3	G	1505	0	1396	54	0
4	D	1891	0	1787	46	0
4	H	1879	0	1767	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9790	0	9139	248	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 13.

The worst 5 of 248 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:18:GLY:O	1:A:75:ARG:NH1	2.12	0.79
4:D:220:TRP:HZ2	4:D:224:ARG:HB3	1.46	0.79
3:G:152:ASP:OD1	3:G:191:ASN:ND2	2.16	0.78
4:H:180:LEU:HB3	4:H:183:SER:HB2	1.64	0.78
3:C:97:THR:HG22	3:C:100:LYS:HB3	1.63	0.78

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	169/180 (94%)	161 (95%)	8 (5%)	0	100	100
1	E	172/180 (96%)	163 (95%)	9 (5%)	0	100	100
2	B	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	F	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	C	189/212 (89%)	181 (96%)	8 (4%)	0	100	100
3	G	193/212 (91%)	181 (94%)	12 (6%)	0	100	100
4	D	237/243 (98%)	225 (95%)	12 (5%)	0	100	100
4	H	237/243 (98%)	227 (96%)	10 (4%)	0	100	100
All	All	1211/1288 (94%)	1149 (95%)	62 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	142/148 (96%)	140 (99%)	2 (1%)	69	90
1	E	143/148 (97%)	138 (96%)	5 (4%)	39	73
2	B	7/7 (100%)	7 (100%)	0	100	100
2	F	7/7 (100%)	7 (100%)	0	100	100
3	C	166/186 (89%)	156 (94%)	10 (6%)	21	52
3	G	164/186 (88%)	155 (94%)	9 (6%)	24	56
4	D	205/208 (99%)	194 (95%)	11 (5%)	24	57
4	H	203/208 (98%)	195 (96%)	8 (4%)	35	70
All	All	1037/1098 (94%)	992 (96%)	45 (4%)	32	66

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	215	SER
1	E	58	GLU
4	H	57	ILE
4	D	228	VAL
1	E	92	THR

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 [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	173/180 (96%)	-0.23	1 (0%) 89 89	39, 75, 121, 148	0
1	E	174/180 (96%)	-0.08	4 (2%) 60 58	39, 77, 150, 167	0
2	B	9/9 (100%)	0.00	1 (11%) 5 4	49, 60, 78, 88	0
2	F	9/9 (100%)	-0.30	0 100 100	62, 71, 88, 92	0
3	C	195/212 (91%)	-0.21	4 (2%) 63 61	32, 82, 143, 184	0
3	G	197/212 (92%)	-0.28	2 (1%) 82 81	34, 75, 131, 182	0
4	D	239/243 (98%)	-0.26	2 (0%) 86 85	35, 68, 120, 145	0
4	H	239/243 (98%)	-0.29	0 100 100	33, 72, 111, 158	0
All	All	1235/1288 (95%)	-0.23	14 (1%) 80 80	32, 74, 128, 184	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	17	LEU	6.2
3	C	137	LEU	5.1
1	A	16	GLY	4.2
3	G	0	ALA	3.9
1	E	16	GLY	3.5

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.